Electronic Supporting Information

Equatorial ligand plane perturbations lead to a spin-state change in an iron(III) porphyrin dimer

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Part 1: Experimental and computational methods

Experimental Section

Trans-1,2-bis[(chloro){5-(2,3,7,8,12,13,17,18-octaethylporphyrinyl)}iron(III)]ethane, **2**•Cl was prepared by modifying the literature methods.[1] Reagents and solvents were purchased from commercial sources and purified by standard procedures.

Synthesis of 2•perchlorate: 100 mg of **2**•Cl (0.079 mmol) was dissolved in 40 mL benzene and 33 mg (0.158 mmol) $AgClO_4$ in 2 mL acetonitrile was added to it and stirred at room temperature for 1hour. The resulting solution was then evaporated to complete dryness. The solid was then dissolved in dichloromethane and the insoluble AgCl was filtered off. The filtrate thus obtained was then evaporated to dryness. The resulting solid was dissolved in minimum volume of dry CH_2Cl_2 and then carefully layered with benzene. On standing for 4–5 days, dark brown crystalline solid was formed which was collected by filtration and dried in vacuum. Yield: 90 mg (81%). ***Caution!*** *Perchlorate salts are potentially explosive when heated or shocked. Handle them in milligram quantities with care.* Yield: 91 mg, (77%). Anal. Calcd (found): C, 63.48 (63.70); H, 6.37 (6.55); N, 8.00 (8.15). UV-vis (dichloromethane) [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 394 (1.4×10^5), 492 (3.1×10^4), 545 (1.1×10^4), 640 (5.1×10^3). ^{1}H NMR ($CDCl_3$, 295 K): *meso-H*: –3.9, –15.7; –C*H*$_3$: 2.6, 2.7, 2.8; –C*H*$_2$: 16.0, 16.7, 17.2, 17.9, 18.1, 18.7, 19.2, 21.4; –C*H*(b): 33.6 ppm. Mössbauer: (α-Fe, 295 K): δ= 0.28 mm s^{-1}, ΔE_Q= 2.67 mm s^{-1}.

Synthesis of 2•picrate: 100 mg (0.079 mmol) of **2**•Cl was dissolved in 50 mL dichloromethane. 40 mg (0.174 mmol) 2,4,6-trinitrophenol in 2 mL dichloromethane was added to it and the was then refluxed for 30 min. The resulting solution was evaporated to complete dryness. The solid thus obtained was dissolved in minimum volume of dichloromethane, filtered to remove any solid residue and carefully layered with acetonitrile which was then kept for slow diffusion in air at room temperature. On standing for 5–6 days, dark brown crystalline solid was formed which was then collected by filtration, washed well with the mother liquor and dried in vacuum. Yield: 98 mg, (75%). Anal. Calcd (found): C, 62.32 (62.51); H, 5.59 (5.75); N, 11.83 (11.95). UV-vis (dichloromethane) [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 368 (1.9×10^5), 516 (2.8×10^4), 547 (2.2×10^4), 653 (1.1×10^4). EPR data: in solid (120 K), $g_\perp$= 6.02 and $g_\parallel$= 2.01; in dichloromethane (120 K), $g_\perp$=

6.05 and $g_{\|}$= 1.97.^{1}H NMR ($CDCl_3$, 295 K): *meso-H*: –22.0, –43.7;–CH_3: 5.9, 6.7, 7.7, 8.4; –CH_2: 35.5, 38.2, 39.1, 50.2, 51.5, 51.9, 53.2, 55.4; –CH_2(b): 109.5; m_t *-H*: 52.4 ppm. Mössbauer: (α-Fe, 295 K): δ= 0.30 mm s^{-1}, ΔE_Q= 0.58 mm s^{-1}.

Instrumentation

UV-vis spectra were recorded on a PerkinElmer UV/Vis spectrometer. ^{57}Fe Mössbauer spectra were recorded using a Wissel 1200 spectrometer and a proportional counter. ^{57}Co(Rh) in a constant acceleration mode was used as the radioactive source. Isomer shifts (δ) are given related to α-iron foil at room temperature. Elemental (C, H, and N) analyses were performed on a PerkinElmer 2400II elemental analyzer. Electron paramagnetic resonance (EPR) spectra were obtained on a Bruker EMX EPR spectrometer. EPR spectral simulations were carried out using the Easy Spin software.[2] Magnetic susceptibility data were collected using a Quantum Design MPMS SQUID magnetometer over the temperature range 5 to 300K. Data were collected in applied magnetic field of 0.2 T and corrected for diamagnetism using Pascal's constants. ^{1}H NMR spectra were recorded on a JEOL 500 MHz instrument. The spectra for paramagnetic molecules were recorded over a 100-kHz bandwidth with 64 K data points and a 5-ms 90° pulse. For a typical spectrum between 2000 and 3000 transients were accumulated with a 50-μs delay time. The residual ^{1}H resonances of the solvents were used as a secondary reference.

X-ray Structure Solution and Refinement

Single-crystal X-ray data were collected at 100 K on a Bruker SMART APEX CCD diffractometer equipped with CRYO Industries low temperature apparatus and intensity data were collected using graphite-monochromated MoKα radiation (λ= 0.71073 Å). The data integration and reduction were processed with SAINT software.[3] An absorption correction was applied.[4] The structure was solved by the direct method using SHELXS-97 and was refined on F2 by full-matrix least-squares technique using the SHELXL-2014 program package.[5] Non-hydrogen atoms were refined anisotropically. In the refinement, hydrogens were treated as riding atoms using SHELXL default parameters. Crystal data and data collection parameters are given in Table S2.

Computational modeling

Following previously benchmarked methods,[6] we utilized the OPBE[7] density functional theory (DFT) method for geometry optimizations and frequencies in the gas phase for structures **1•**X**, 2•**X**, 1A•**X**, 2A•**X with perchlorate and picrate as axial ligand (X). Thus, our initial calculations utilized an abbreviated system with all substituents of the two porphyrin residues set to hydrogen atoms (models **1A•**Xand **2A•**X representing the ethane-bridged and ethene-bridged dimers, respectively). In addition, we studied the full models (models **1•**X and **2•**X, Scheme S1) for a selection of methods and spin states. All structures were geometry minimized without constraints using a double-ζ quality LACVP basis set on iron with electron core-potential and 6-31G* on the rest of the atoms: basis set BS1.[8] All calculations are the result of a full geometry optimization on the overall $S = 1$ spin states with individual metal spin state $S = (^3/_2, -^3/_2)$ or $S = (^5/_2, -^5/_2)$ and a frequency calculation confirms the structures as local minima. In addition, the maximum (ferromagnetic) spin states were calculated as well, i.e. $S = (^3/_2, ^3/_2)$ and $S = (^5/_2, ^5/_2)$. All calculations for complexes **1•**X**, 2•**X**, 1A•**X**, 2A•**X were run in Gaussian-09.[9]

To test the effect of spin state on structure, model size, energetics and environmental factors, we ran a number of exploratory calculations on models**1A•**X and **2A•**X with the BS1 basis set. Firstly, the effect of the density functional methods on the relative energies of the spin state ordering of the $S = (^3/_2, ^3/_2)$, $(^3/_2, ^5/_2)$ and $(^5/_2, ^5/_2)$ spin states was investigated through full geometry optimizations at the OPBE,[7] PBE0,[10] B98,[11] and BP86[12] functionals in the presence of an implicit solvent model mimicking water. In all cases the same spin-state ordering is obtained, although there is some fluctuation in the relative energies. In addition, inclusion of a solvent model does not affect the spin state energies with respect to the gas-phase either.

On some structures, the energetics was improved by single point calculations on all structures using the 6-311+G** basis set for all atoms: basis set BS2. Finally a single point using basis set def2-TZVP with the functional TPSSh[13] was performed on all geometries: BS3.

References:

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Part 2: Experimental data

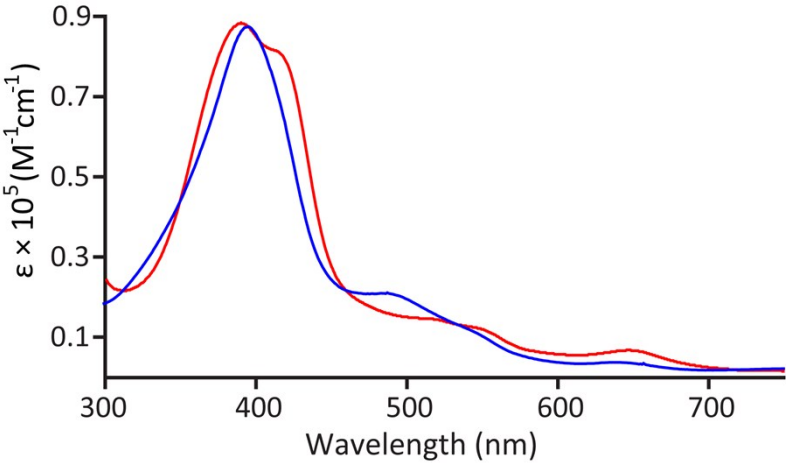


Fig. S1. UV-visible spectra (in dichloromethane at 295 K) of **1**•perchlorate (red line), and **2**•perchlorate (blue line).

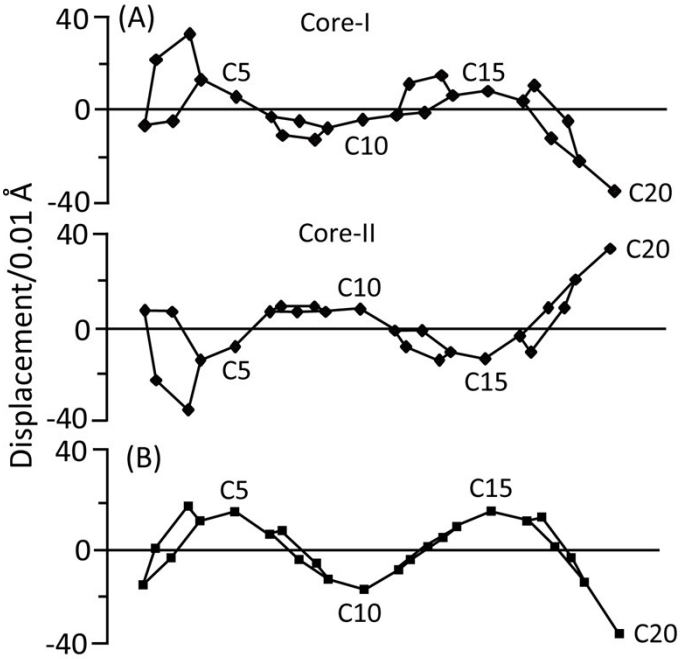


Fig. S2. Out-of-plane displacements (in units of 0.01 Å) of the porphyrin core atoms of (A) **1**•perchlorate, and (B) **2**•perchlorate from the mean plane of the $C_{20}N_4$ porphyrinato core. The horizontal axes show the bond connectivity between atoms.

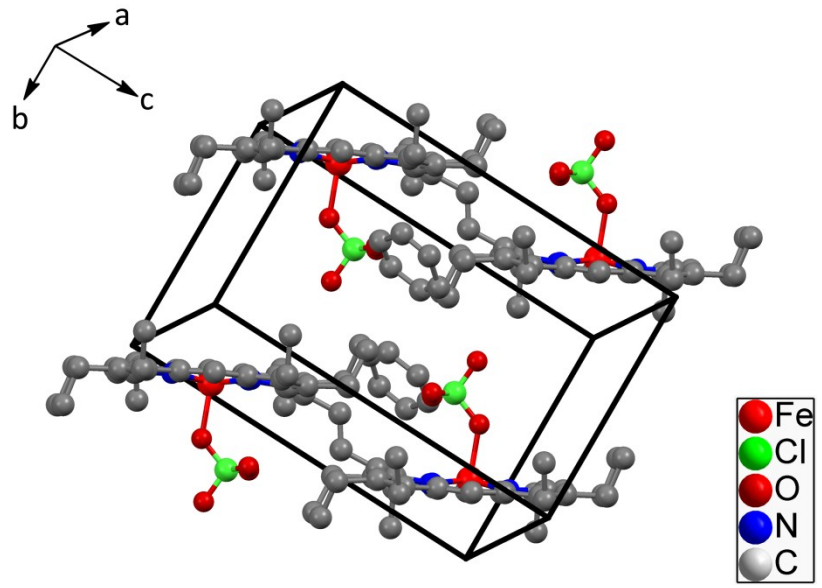


Fig. S3. Diagram illustrating the molecular packing of **2**•perchlorate.$2C_6H_6$ at 100 K (hydrogen atoms have been omitted for clarity).

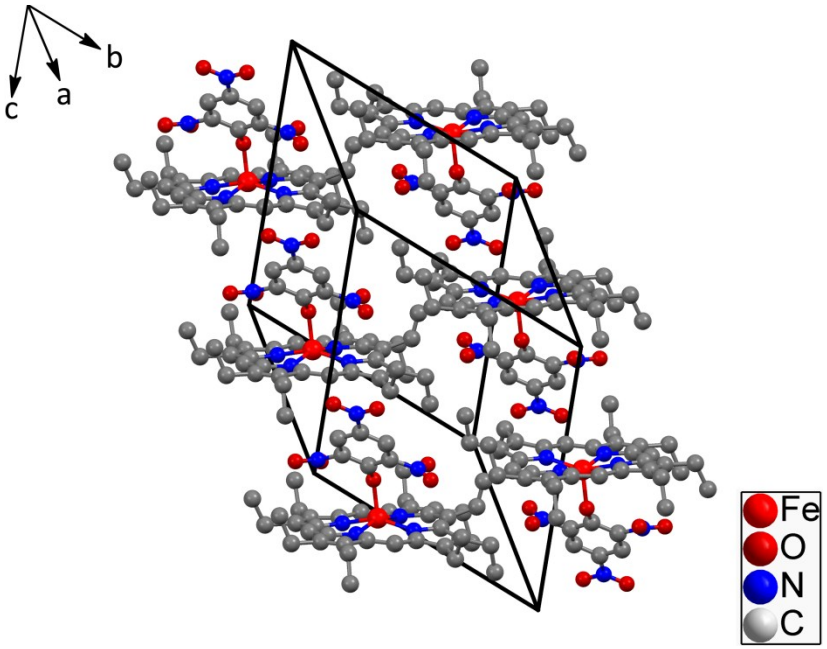


Fig. S4. Diagram illustrating the molecular packing of **2**•picrate at 100 K (hydrogen atoms have been omitted for clarity).

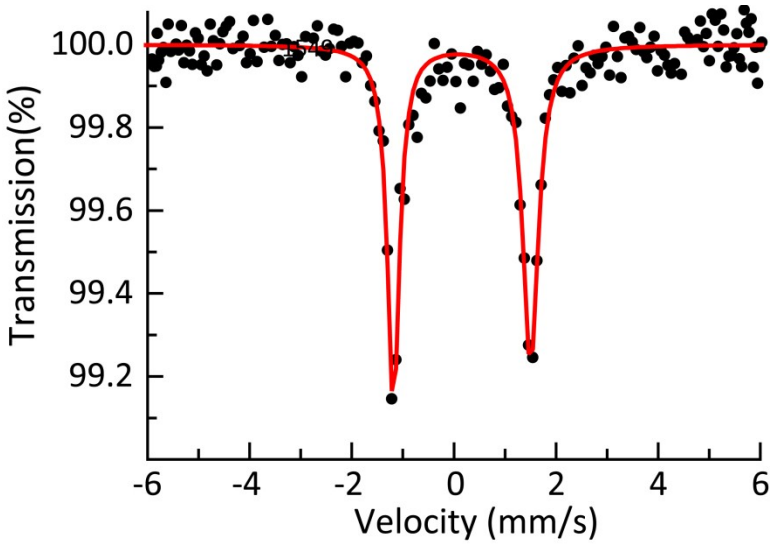


Fig. S5. Zero-field Mössbauer spectrum (at 100 K) of microcrystalline sample of **2**•perchlorate.

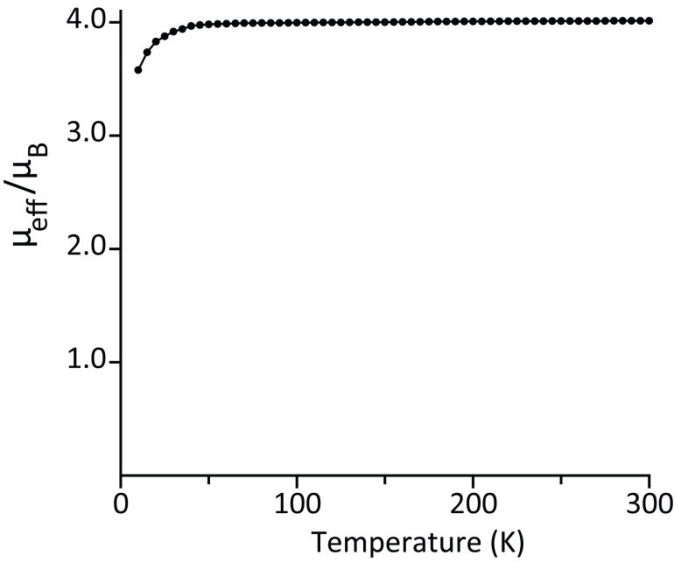


Fig. S6. Magnetic moment per iron center of crystalline sample of **2**•perchlorate as a function of temperature.

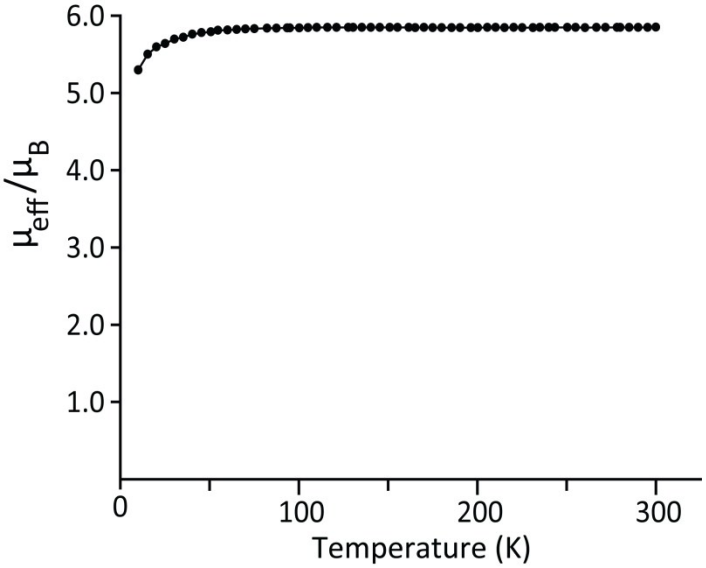


Fig. S7. Magnetic moment per iron center of crystalline sample of **2**•picrate as a function of temperature.

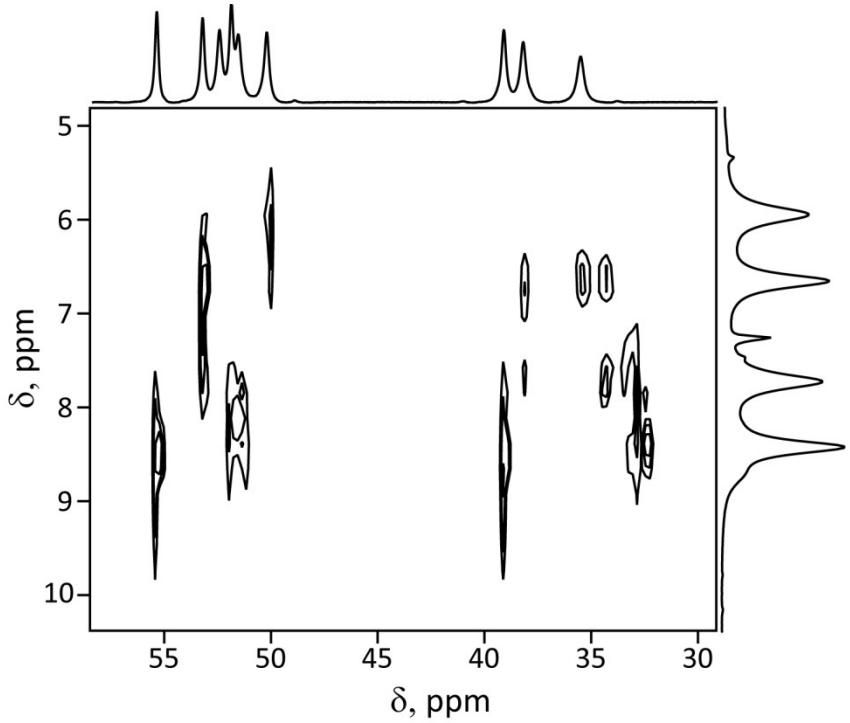


Fig. S8. $^{1}H - {}^{1}H$ COSY (500 MHz) spectrum (in $CDCl_3$ at 295 K) of **2**•picrate.

Table S1. Selected Bond Distances (Å) and Bond angles (°)

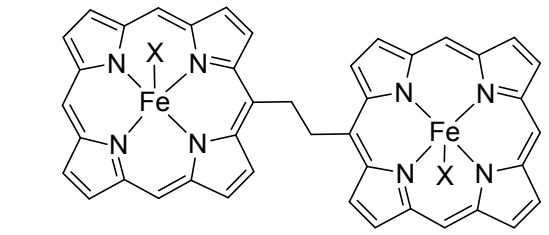
Bond distances	**2**•perchlorate.2C_6H_6	**2**•picrate
Fe1–N1	1.989(4)	2.037(3)
Fe1–N2	2.000(4)	2.044(3)
Fe1–N3	2.003(4)	2.056(3)
Fe1–N4	2.004(4)	2.051(3)
Fe1–O1	2.056(4)	1.915(3)
N1–Fe1–N2	90.00(16)	89.01(13)
N1–Fe1–N3	165.36(16)	160.25(14)
N1–Fe1–N4	87.80(16)	86.89(13)
N2–Fe1–N3	88.08(16)	87.25(14)
N2–Fe1–N4	165.43(17)	155.81(14)
N3–Fe1–N4	90.42(16)	88.61(13)
N1–Fe1–O1	102.08(15)	102.76(12)
N2–Fe1–O1	95.56(15)	99.13(13)
N3–Fe1–O1	92.55(15)	96.98(13)
N4–Fe1–O1	98.99(15)	105.03(13)

Table S2. Crystallographic Data and Data Collection Parameters

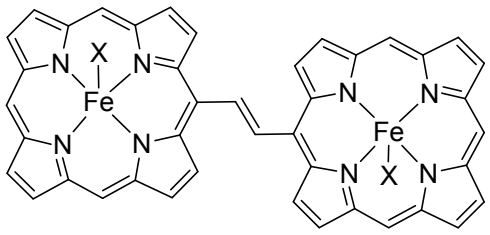
	2•perchlorate.2C_6H_6	**2**•picrate
Formula	$C_{86}H_{100}Cl_2Fe_2N_8O_8$	$C_{86}H_{92}Fe_2N_{14}O_{14}$
T (K)	100(2)	100(2)
Formula weight	1556.33	1657.43
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a, Å	10.8619(12)	12.077(5)
b, Å	13.5788(15)	13.443(5)
c, Å	15.2373(18)	14.103(5)
α, deg	64.626(2)	62.358(5)
β, deg	78.507(2)	74.156(5)
γ, deg	71.060(2)	72.733(5)
V, Å^3	1915.9(4)	1912.0(13)
Z	1	1
Radiation (λ, Å)	Mo Kα (0.71073)	Mo Kα (0.71073)
d_{calcd}, g•cm^{-3}	1.349	1.439
F(000)	822	870
Crystal size (mm^3)	0.26 x 0.20 x 0.16 mm^3	0.18 x 0.14 x 0.10 mm^3
Theta range for data collection	1.724 to 25.497°	2.236 to 25.498°
μ, mm^{-1}	0.512	0.458
No of unique data	7006	7129
Completeness to theta	98.4%	99.7%
No. of restraints	0	0
No. of params. refined	486	531
GOF on F^2	1.027	1.039
$R1$[a] [$I > 2\sigma(I)$]	0.0691	0.0664
$R1$[a](all data)	0.1106	0.1112
w$R2$[b] (all data)	0.1998	0.1770
Largest diff. peak and hole	1.118 and –0.738 eÅ^{-3}	1.271 and –0.384 eÅ^{-3}

$$^{a}R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|} \quad ; \; ^{b}wR2 = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right)^2\right]}{\sum \left[w\left(F_o^2\right)^2\right]}}$$

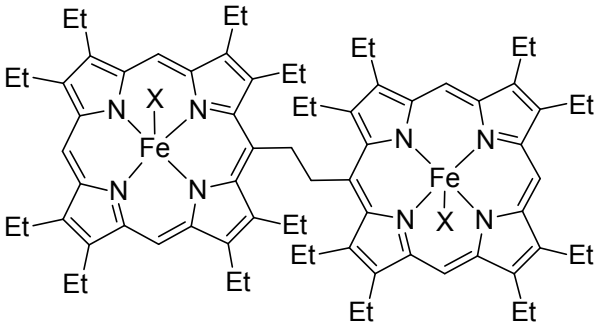
Part 3: Computational Studies:



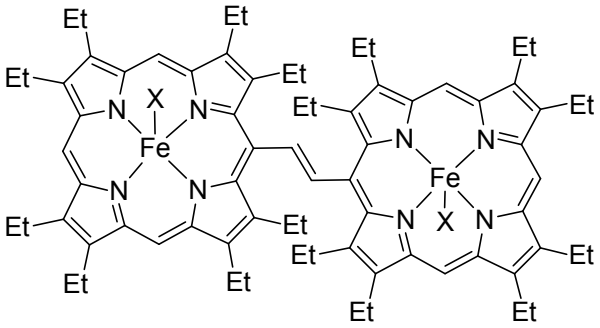
1A·X



2A·X



1·X



2·X

X= ClO_4, picrate

Scheme S1: Models investigated in this work.

Part 3A: Small Model with Perchlorate Ligand

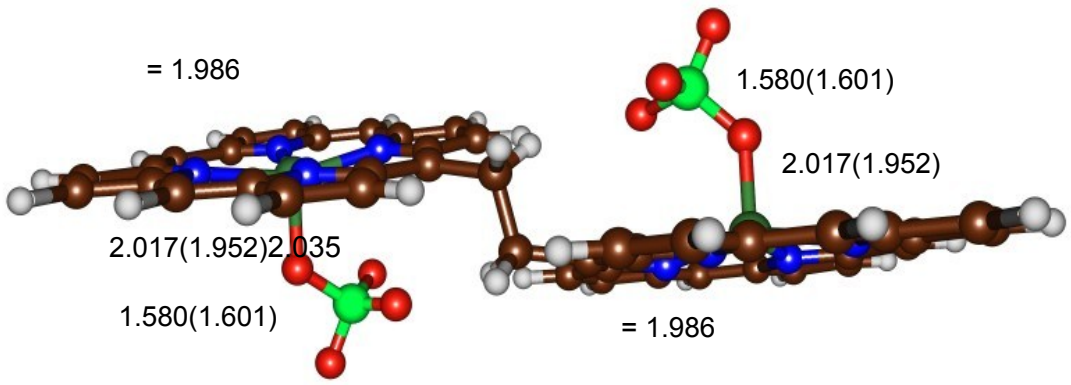


Fig. S9. Optimized geometries (distances in Å) in the gas phase of ^{1}**1A•**perchlorate {3/2} (^{1}**1A•**perchlorate {5/2}) as obtained at UOPBE/BS1 in Gaussian.

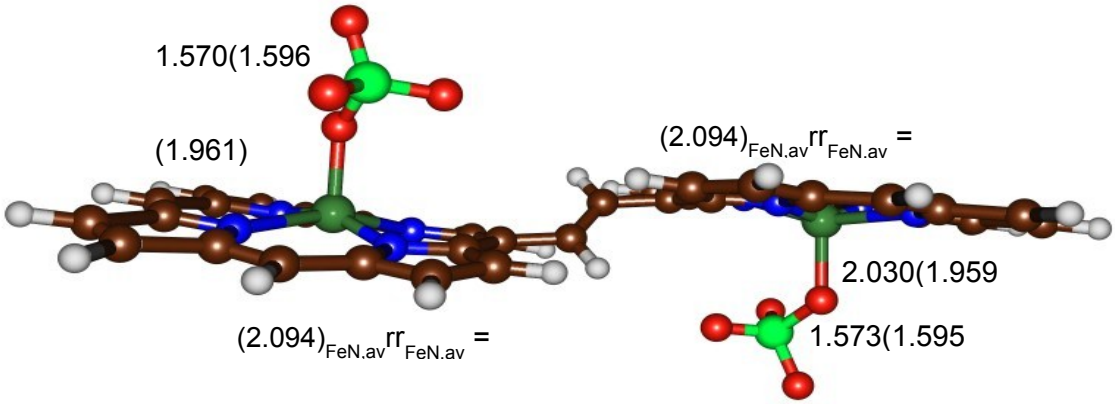


Fig. S10. Optimized geometries (distances in Å) of ^{1}**2A•**perchlorate {3/2} (^{1}**2A•**perchlorate {5/2})as obtained at UOPBE/BS1 in Gaussian.

Table S3: Absolute [in au] and relative [in kcal mol^{-1}] energies of optimized spin state structures as calculated at OPBE/BS1, OPBE/BS2, and TPSSh/BS3. Data obtained in the gas-phase.

(a) OPBE/BS1 data:

BS1	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{1}**1A**•perchlorate {3/2}	-3822.009934	-3821.395840	-3821.485220	0.00	0.00	0.28
^{1}**1A**•perchlorate {5/2}	-3822.005089	-3821.394429	-3821.485669	3.04	0.89	0.00
^{1}**2A**•perchlorate {3/2}	-3820.784618	-3820.195120	-3820.284860	0.00	0.00	1.04
^{1}**2A**•perchlorate {5/2}	-3820.780653	-3820.194476	-3820.286520	2.49	0.40	0.00

(b) OPBE/BS2 data:

BS2	E [au]	ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{1}**1A**•perchlorate {3/2}	-6103.788366	-6103.174272	-6103.263652	0.00	0.00	0.00
^{1}**1A**•perchlorate {5/2}	-6103.782618	-6103.171958	-6103.263198	3.61	1.45	0.28
^{1}**2A**•perchlorate {3/2}	-6102.563591	-6101.974093	-6102.063833	0.00	0.00	0.00
^{1}**2A**•perchlorate {5/2}	-6102.557402	-6101.971225	-6102.063269	3.88	1.80	0.35

(c) TPSSh/BS3 data:

BS3	E [au]	ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{1}**1A**•perchlorate {3/2}	-6104.703442	-6104.089348	-6104.178728	0.00	0.00	0.00
^{1}**1A**•perchlorate {5/2}	-6104.680502	-6104.069842	-6104.161082	14.39	12.24	11.07
^{1}**2A**•perchlorate {3/2}	-6103.476286	-6102.886789	-6102.976529	0.00	0.00	0.00
^{1}**2A**•perchlorate {5/2}	-6103.451814	-6102.865637	-6102.957681	15.36	13.27	11.83

Table S4: Absolute [in au] and relative [in kcal mol^{-1}] energies of optimized spin state structures as calculated at OPBE/BS1, PBE0/BS1, B98/BS1, and BP86/BS1. Data obtained with a dielectric constant mimicking water included.

OPBE/BS1	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{11}**1A**•perchlorate	-3822.04828	-3821.43825	-3821.53237	8.40	6.17	5.67
^{9}**1A**•perchlorate	-3822.05492	-3821.44278	-3821.53472	4.23	3.33	4.20
^{7}**1A**•perchlorate	-3822.06166	-3821.44808	-3821.54140	0.00	0.00	0.00
^{11}**2A**•perchlorate	-3820.82511	-3820.23890	-3820.32982	8.26	6.40	6.86
^{9}**2A**•perchlorate	-3820.83222	-3820.24432	-3820.33541	3.80	2.99	3.35
^{7}**2A**•perchlorate	-3820.83827	-3820.24909	-3820.34076	0.00	0.00	0.00

PBE0/BS1	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{11}**1A**•perchlorate	-3819.30867	-3818.68249	-3818.77351	7.86	5.68	4.19
^{9}**1A**•perchlorate	-3819.31505	-3818.68707	-3818.77668	3.86	2.81	2.19
^{7}**1A**•perchlorate	-3819.32121	-3818.69155	-3818.78018	0.00	0.00	0.00
^{11}**2A**•perchlorate	-3818.08520	-3817.48352	-3817.57443	7.61	5.53	3.98
^{9}**2A**•perchlorate	-3818.09155	-3817.48819	-3817.57629	3.62	2.60	2.81
^{7}**2A**•perchlorate	-3818.09732	-3817.49233	-3817.58077	0.00	0.00	0.00

B98/BS1	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{11}**1A**•perchlorate	-3821.44193	-3820.82842	-3820.92004	20.60	15.87	14.85
^{9}**1A**•perchlorate	-3821.45838	-3820.84190	-3820.93138	10.28	7.41	7.73
^{7}**1A**•perchlorate	-3821.47476	-3820.85370	-3820.94370	0.00	0.00	0.00
^{11}**2A**•perchlorate	-3820.21698	-3819.62535	-3819.71385	19.27	16.11	16.38
^{9}**2A**•perchlorate	-3820.23443	-3819.64138	-3819.73100	8.32	6.05	5.62
^{7}**2A**•perchlorate	-3820.24769	-3819.65102	-3819.73996	0.00	0.00	0.00

BP86/BS1	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{11}**1A**•perchlorate	-3822.94790	-3822.35107	-3822.44766	30.40	27.32	24.65
^{9}**1A**•perchlorate	-3822.97196	-3822.37225	-3822.46492	15.30	14.03	13.81
^{7}**1A**•perchlorate	-3822.99634	-3822.39461	-3822.48693	0.00	0.00	0.00
^{11}**2A**•perchlorate	-3821.72747	-3821.15386	-3821.24940	29.89	27.25	24.81
^{9}**2A**•perchlorate	-3821.75172	-3821.17590	-3821.26858	14.67	13.42	12.77
^{7}**2A**•perchlorate	-3821.77511	-3821.19729	-3821.28893	0.00	0.00	0.00

Part 3B: Small Model with picrate Ligand

Table S5: Absolute [in au] and relative [in kcal mol^{-1}] energies of optimized spin state structures as calculated at OPBE/BS1, and picrate ligand.

BS1	E [au]	ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{11}**1A**•picrate	-4140.825627	0.777478	-4140.166590	0.58	-1.38	-3.24
^{1}**1A**•picrate{3/2}	-4140.826546	0.780600	-4140.161432	0.00	0.00	0.00
^{7}**1A**•picrate	-4140.828906	0.780389	-4140.161771	-1.48	-1.61	-0.21
^{11}**2A**•picrate	-4139.607226	0.753557	-4138.970051	0.22	-1.56	-4.60
^{1}**2A**•picrate{3/2}	-4139.607581	0.756406	-4138.962716	0.00	0.00	0.00
^{7}**2A**•picrate	-4139.608106	0.756675	-4138.965073	-0.33	-0.16	-1.48

Part 3C: Large Model with perchlorate Ligand

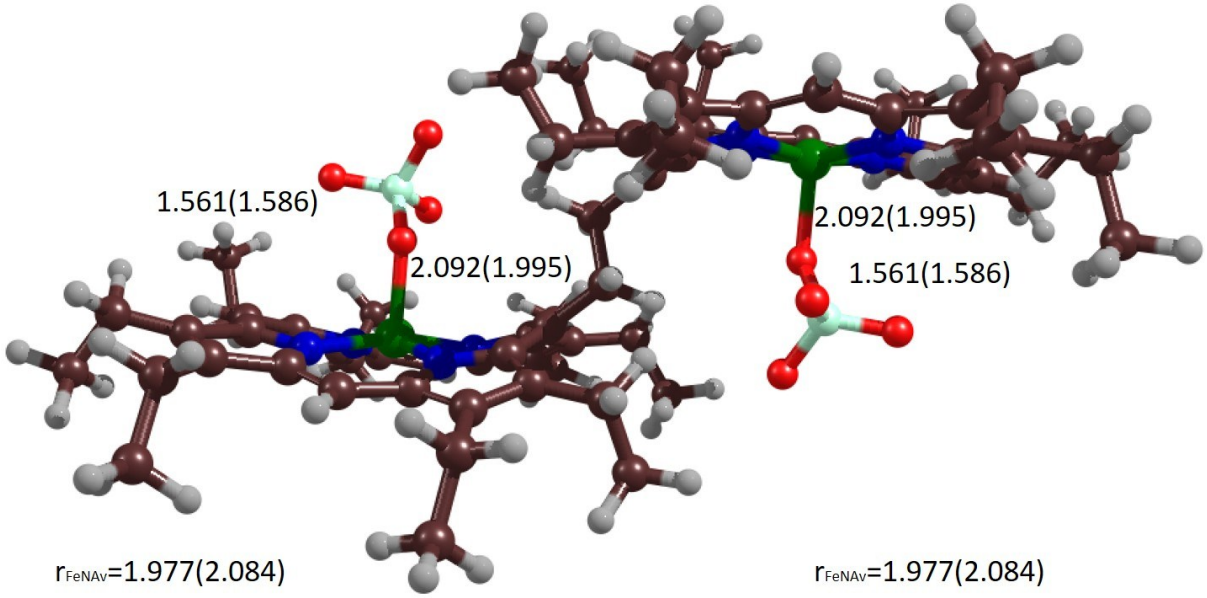


Fig. S11: Optimized geometries (distances in Å) of ^{1}**1**•perchlorate {3/2} (^{1}**1**•perchlorate {5/2}) as obtained at UOPBE/BS1 in Gaussian.

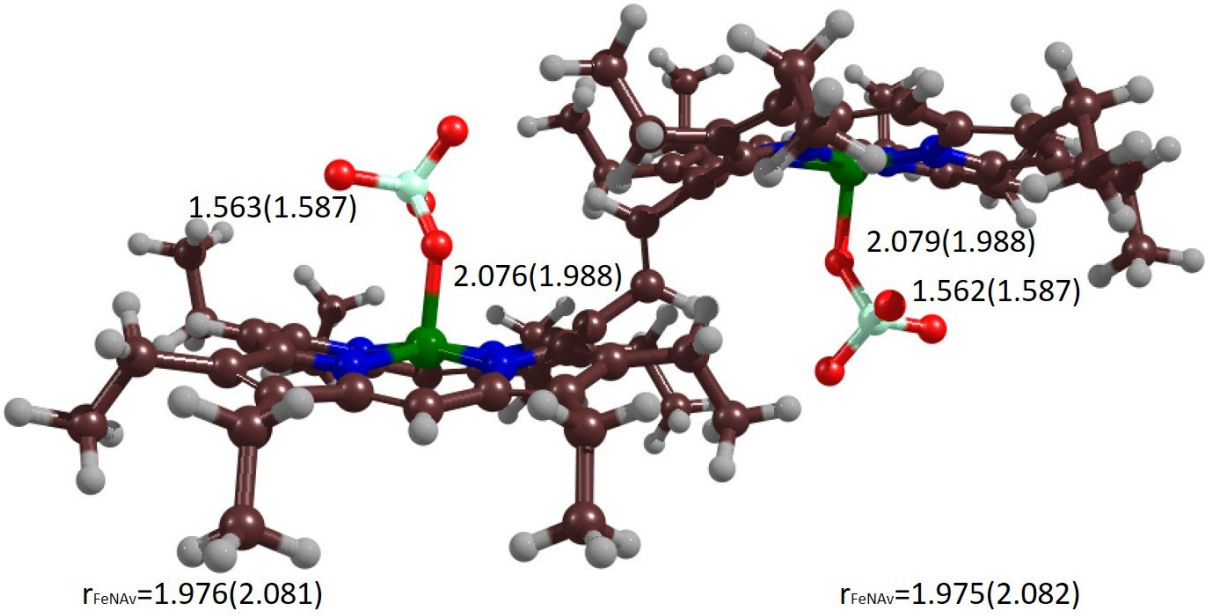


Fig. S12: Optimized geometries (distances in Å) of ^{1}**2**•perchlorate {3/2} (^{1}**2**•perchlorate {5/2}) as obtained at UOPBE/BS1 in Gaussian.

Table S6: Absolute [in au] and relative [in kcal mol^{-1}] energies of optimized spin state structures as calculated at OPBE/BS1, OPBE/BS2, and TPSSh/BS3.

BS1	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{1}**1**•perchlorate {3/2}	-5079.50983	-5077.99619	-5078.14247	0.00	0.00	0.00
^{1}**1**•perchlorate {5/2}	-5079.49975	-5077.98921	-5078.13594	6.32	4.38	4.10
^{1}**2**•perchlorate {3/2}	-5078.29344	-5076.80411	-5076.94707	0.00	0.00	0.00
^{1}**2**•perchlorate {5/2}	-5078.28304	-5076.79778	-5076.94412	6.53	3.98	1.85

BS2	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{1}**1**•perchlorate {3/2}	-7361.683904	-7360.170266	-7360.316544	0.00	0.00	0.00
^{1}**1**•perchlorate {5/2}	-7361.673236	-7360.162690	-7360.309422	6.69	4.75	4.47
^{1}**2**•perchlorate {3/2}	-7360.466726	-7358.977405	-7359.120364	0.00	0.00	0.00
^{1}**2**•perchlorate {5/2}	-7360.456147	-7358.970889	-7359.117234	6.64	4.09	1.96

BS3	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{1}**1**•perchlorate {3/2}	-7363.289879	-7361.776241	-7361.922519	0.00	0.00	0.00
^{1}**1**•perchlorate {5/2}	-7363.260224	-7361.749679	-7361.896411	18.61	16.67	16.38
^{1}**2**•perchlorate {3/2}	-7362.070036	-7360.580715	-7360.723674	0.00	0.00	0.00
^{1}**2**•perchlorate {5/2}	-7362.041724	-7360.556466	-7360.702811	17.77	15.22	13.09

Part 3D: Large Model with picrate Ligand

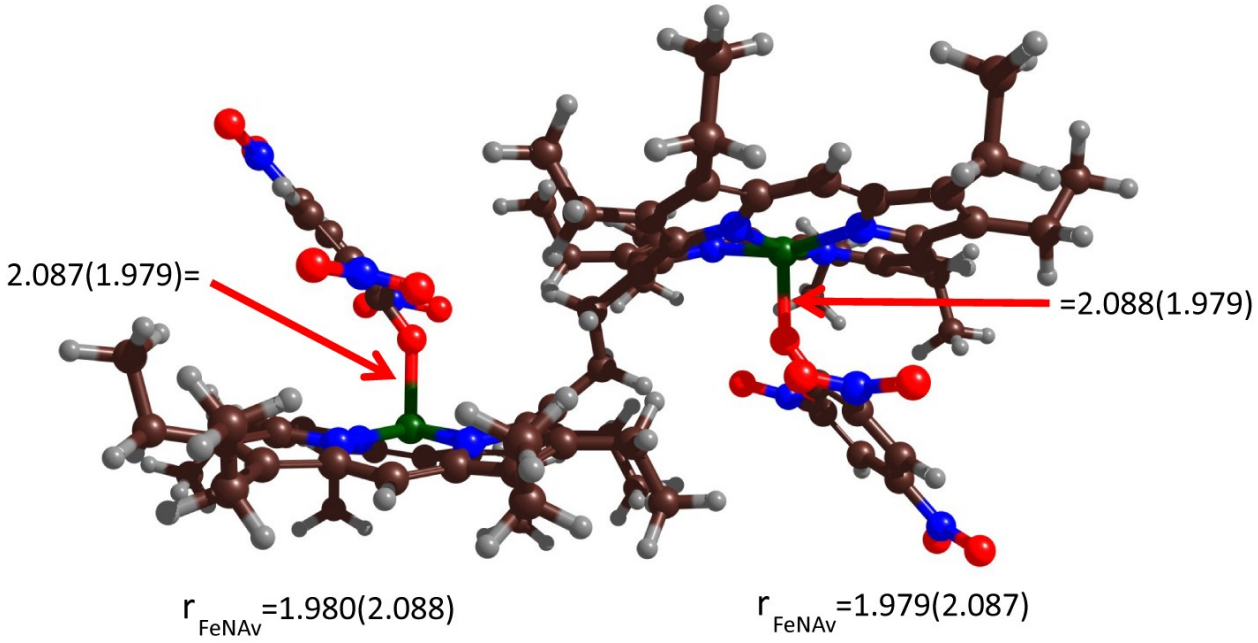


Fig. S13: Optimized geometries (distances in Å) of ^{7}**1**•picrate (^{11}**1**•picrate) as obtained at UOPBE/BS1 in Gaussian.

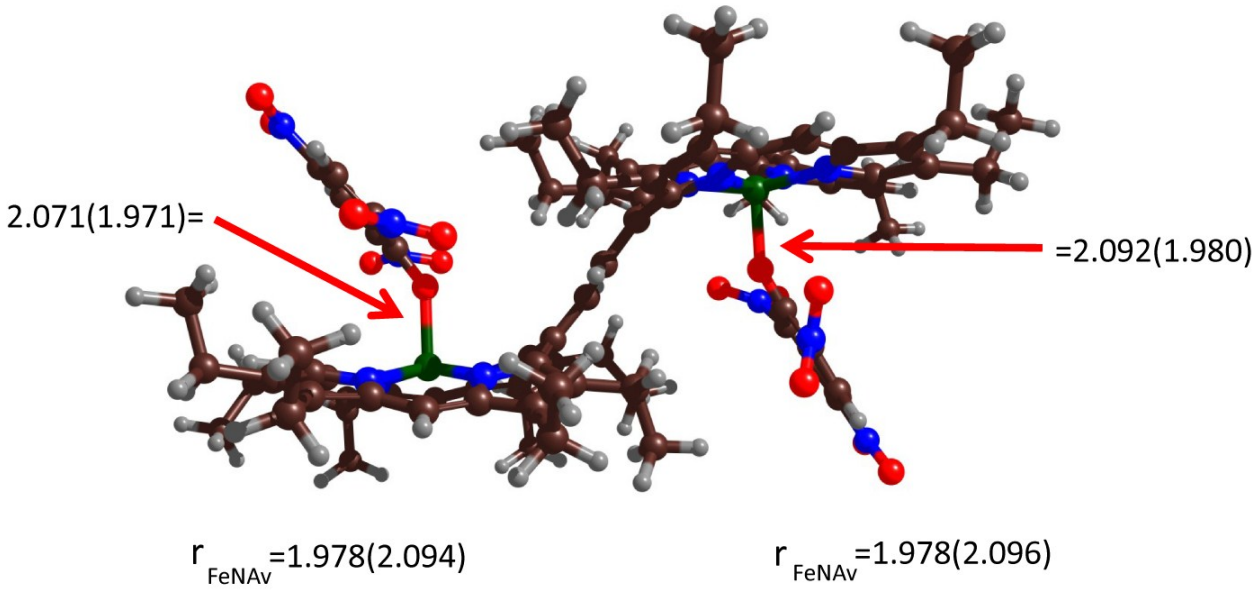


Fig. S14: Optimized geometries (distances in Å) of ^{7}**2**•picrate (^{11}**2**•picrate) as obtained at UOPBE/BS1 in Gaussian

Table S7: Absolute [in au] and relative [in kcal mol^{-1}] energies of optimized spin state structures as calculated at OPBE/BS1 with picrate axial ligand.

BS1	E [au]	E+ZPE [au]	G [au]	ΔE	ΔE+ZPE	ΔG
^{11}**1**•picrate	-5398.321982	1.677826	-5396.817277	5.51	3.61	0.11
^{1}**1**•picrate{3/2}	-5398.330768	1.680855	-5396.817454	0.00	0.00	0.00
^{7}**1**•picrate	-5398.330681	1.681025	-5396.815255	0.05	0.16	1.38
^{11}**2**•picrate	-5397.112488	1.652628	-5395.632828	3.59	1.44	-1.31
^{1}**2**•picrate{3/2}	-5397.118212	1.656059	-5395.630740	0.00	0.00	0.00
^{7}**2**•picrate	-5397.118031	1.656289	-5395.631338	0.11	0.26	-0.38

Part 4: Computation: Cartesian coordinates

Structure ^{1}1A•perchlorate {3/2}

Fe	5.879669000	4.638006000	1.925337000
Fe	6.810756000	-4.440136000	-2.107909000
Cl	7.428969000	2.323777000	3.826597000
N	4.739160000	3.198727000	1.165020000
N	4.343960000	5.278728000	3.053695000
N	6.790817000	6.387315000	2.319291000
N	7.151302000	4.302527000	0.430205000
O	6.798598000	3.722721000	3.494183000
O	6.383072000	1.303497000	3.633924000
O	8.561813000	2.117890000	2.911043000
C	5.126230000	2.172841000	0.320817000
C	4.036603000	1.250313000	0.139694000
C	2.982160000	1.733066000	0.859257000
C	3.434619000	2.920403000	1.514149000
C	2.655820000	3.624973000	2.420922000
H	1.644035000	3.265676000	2.598386000
C	3.100944000	4.704166000	3.167375000
C	2.339682000	5.339061000	4.205553000
C	3.149302000	6.293753000	4.753041000
C	4.383051000	6.258261000	4.018719000
C	5.427680000	7.150670000	4.210855000
H	5.340102000	7.877228000	5.016238000
C	6.532188000	7.231153000	3.374294000
C	7.519674000	8.271080000	3.443820000
C	8.374653000	8.070255000	2.396963000
C	7.922228000	6.888179000	1.720482000
C	8.571832000	6.310150000	0.641419000
H	9.456937000	6.810361000	0.253234000
C	8.217681000	5.097080000	0.067664000
C	8.988746000	4.464885000	-0.957264000
C	8.413563000	3.247586000	-1.185378000
C	7.264291000	3.154103000	-0.328071000
C	6.364761000	2.076701000	-0.332557000
C	6.748432000	0.788635000	-1.019082000
H	7.258025000	0.978384000	-1.971068000
H	5.859638000	0.212422000	-1.286134000
O	7.851896000	2.426325000	5.225795000
H	1.984185000	1.313373000	0.948288000
H	1.324082000	5.070815000	4.483123000
H	2.933357000	6.978917000	5.568198000
H	7.536052000	9.060327000	4.190392000
H	9.867147000	4.895477000	-1.429749000
H	8.730648000	2.501900000	-1.905216000
C	10.021464000	-1.906935000	-3.234369000
H	4.033956000	0.365051000	-0.485725000
Cl	3.940599000	-2.918306000	-2.897483000
C	8.481843000	-5.076054000	-4.570052000
C	8.482987000	-5.911814000	-5.737805000
C	7.390520000	-6.727674000	-5.636737000
C	6.762336000	-6.421566000	-4.382446000
C	5.706460000	-7.141961000	-3.837612000
H	5.254042000	-7.926566000	-4.440603000
C	5.294546000	-7.008127000	-2.518578000
C	4.418166000	-7.924552000	-1.846020000
C	4.392736000	-7.551274000	-0.531037000
C	5.207794000	-6.375152000	-0.420536000
C	5.351793000	-5.622006000	0.735090000
H	4.869673000	-5.980961000	1.642279000
C	5.962962000	-4.375428000	0.780013000
C	5.890596000	-3.498716000	1.908490000
C	6.427793000	-2.304373000	1.519228000
C	6.897815000	-2.476144000	0.169277000
C	7.649010000	-1.528641000	-0.544958000
C	7.656367000	-0.087423000	-0.104043000
H	7.294437000	0.001651000	0.921662000
H	8.671359000	0.328463000	-0.085829000
C	9.372262000	-4.036299000	-4.344627000
H	10.173585000	-3.885317000	-5.065659000
O	5.454478000	-3.298823000	-3.097217000
O	3.911525000	-1.446720000	-2.837735000
O	3.464540000	-3.524861000	-1.647218000
O	3.236864000	-3.438994000	-4.073746000
H	9.216077000	-5.859722000	-6.538129000
H	7.050275000	-7.490689000	-6.331370000
H	3.913295000	-8.761091000	-2.321113000
H	3.851811000	-8.010894000	0.291505000
H	5.454864000	-3.754077000	2.870307000
H	6.525341000	-1.413545000	2.129964000
H	10.867085000	-1.666894000	-3.873043000
H	9.812417000	-0.184552000	-1.884410000
C	8.394696000	-1.917800000	-1.671345000
C	9.472641000	-1.152625000	-2.234592000
H	9.244387000	8.655053000	2.110452000
N	6.606676000	-3.755284000	-0.266361000
N	5.760085000	-6.056578000	-1.638749000

N	7.431034000	-5.402456000	-3.746275000
N	8.274170000	-3.115417000	-2.342491000
C	9.239172000	-3.102505000	-3.323331000

Structure [1]**1A•**perchlorate {5/2}

Fe	6.038630000	4.574587000	2.217414000
Fe	6.573529000	-4.415701000	-2.335179000
Cl	7.437079000	2.217243000	4.074352000
N	4.793264000	3.190393000	1.291268000
N	4.342997000	5.390143000	3.158514000
N	6.875910000	6.493765000	2.446214000
N	7.289818000	4.300219000	0.569398000
O	6.886391000	3.676153000	3.738188000
O	6.303094000	1.293545000	3.945581000
O	8.498366000	1.931341000	3.102332000
C	5.164160000	2.202669000	0.402140000
C	4.068972000	1.276413000	0.231391000
C	3.039306000	1.724493000	1.009596000
C	3.500685000	2.908906000	1.673584000
C	2.733679000	3.634673000	2.585719000
H	1.730789000	3.257318000	2.781783000
C	3.121659000	4.778965000	3.281723000
C	2.307929000	5.480053000	4.241255000
C	3.060664000	6.523451000	4.705536000
C	4.323465000	6.463227000	4.014381000
C	5.354780000	7.393732000	4.149001000
H	5.205766000	8.199462000	4.866780000
C	6.531351000	7.421535000	3.397315000
C	7.526164000	8.461193000	3.459738000
C	8.470023000	8.159584000	2.516340000
C	8.053988000	6.929273000	1.894653000
C	8.748707000	6.269693000	0.881169000
H	9.671603000	6.734457000	0.536323000
C	8.393972000	5.065623000	0.271001000
C	9.168395000	4.431604000	-0.757308000
C	8.532316000	3.261421000	-1.064245000
C	7.355078000	3.184648000	-0.234382000
C	6.401082000	2.143279000	-0.278049000
C	6.739144000	0.891353000	-1.053310000
H	7.215392000	1.133529000	-2.011080000
H	5.829990000	0.348461000	-1.320150000
O	7.930865000	2.326853000	5.445318000
H	2.050397000	1.287841000	1.119082000
H	1.294732000	5.205112000	4.521969000
H	2.785354000	7.275755000	5.439928000
H	7.495533000	9.316014000	4.130118000
H	10.080954000	4.831121000	-1.191402000
H	8.834784000	2.539513000	-1.814469000
C	9.791788000	-1.791161000	-3.559094000
H	4.045590000	0.405072000	-0.413195000
Cl	3.756057000	-2.934239000	-3.129892000
C	8.474339000	-5.184505000	-4.690002000
C	8.619637000	-6.144241000	-5.754144000
C	7.700435000	-7.130893000	-5.521818000
C	7.015410000	-6.779786000	-4.304560000
C	6.063834000	-7.576751000	-3.662852000
H	5.781407000	-8.506012000	-4.155952000
C	5.511398000	-7.331681000	-2.404885000
C	4.671092000	-8.248003000	-1.677030000
C	4.440409000	-7.682873000	-0.453051000
C	5.119238000	-6.412346000	-0.448760000
C	5.109182000	-5.499036000	0.604364000
H	4.557159000	-5.785944000	1.498536000
C	5.697805000	-4.233233000	0.618441000
C	5.585991000	-3.311147000	1.711352000
C	6.220699000	-2.161693000	1.331410000
C	6.755903000	-2.390716000	0.009501000
C	7.567816000	-1.488591000	-0.714568000
C	7.667336000	-0.060080000	-0.234631000
H	7.393466000	0.009362000	0.819995000
H	8.699910000	0.306188000	-0.281525000
C	9.207069000	-4.004128000	-4.568652000
H	9.959784000	-3.812801000	-5.332757000
O	5.174279000	-3.597024000	-3.439604000
O	4.027272000	-1.516269000	-2.859671000
O	3.190730000	-3.626473000	-1.968224000
O	2.982038000	-3.139734000	-4.352535000
H	9.329893000	-6.068007000	-6.573188000
H	7.512382000	-8.024916000	-6.110388000
H	4.320400000	-9.206279000	-2.050879000
H	3.858402000	-8.083428000	0.372598000
H	5.081296000	-3.510991000	2.652610000
H	6.323204000	-1.265033000	1.932520000
H	10.583745000	-1.518982000	-4.251708000
H	9.643736000	-0.084904000	-2.189642000
C	8.277005000	-1.857894000	-1.881128000
C	9.301138000	-1.061381000	-2.512250000
H	9.368216000	8.716377000	2.262842000
N	6.416564000	-3.662095000	-0.406553000
N	5.760660000	-6.215104000	-1.644761000
N	7.491725000	-5.586889000	-3.821260000
N	8.147252000	-3.050437000	-2.553757000
C	9.051449000	-3.021242000	-3.588214000

Structure [1]**2A•**perchlorate {3/2}

Fe	5.976308000	4.762610000	1.974025000
Cl	8.592738000	3.234615000	3.334165000
N	4.692561000	3.286709000	1.641628000
N	4.767599000	5.481791000	3.382309000
N	6.910064000	6.514890000	1.970121000
N	6.802385000	4.310271000	0.229079000
O	7.108843000	3.778036000	3.321577000
O	8.567651000	1.925055000	2.666128000
O	9.436746000	4.200631000	2.618795000
C	4.921014000	2.171775000	0.876734000
C	3.774157000	1.305712000	0.907355000
C	2.846768000	1.908129000	1.713703000
C	3.445041000	3.113160000	2.203077000
C	2.894392000	3.914016000	3.195470000
H	1.919093000	3.633845000	3.589223000
C	3.555962000	4.979409000	3.792682000
C	3.098679000	5.671606000	4.964196000
C	4.068982000	6.579721000	5.288147000
C	5.085478000	6.474515000	4.279901000
C	6.163136000	7.343061000	4.153484000
H	6.312403000	8.092972000	4.927861000
C	6.967438000	7.399919000	3.021835000
C	7.882982000	8.466147000	2.727763000
C	8.348135000	8.246414000	1.460842000
C	7.757090000	7.017518000	1.012506000
C	8.060661000	6.386576000	-0.186214000
H	8.744837000	6.889017000	-0.867352000
C	7.648044000	5.103243000	-0.518567000
C	8.157715000	4.367445000	-1.633954000
C	7.681700000	3.090405000	-1.516320000
C	6.819100000	3.070911000	-0.369688000
C	6.045380000	1.964964000	0.047143000
C	6.382778000	0.635373000	-0.435434000
H	6.797125000	0.550144000	-1.438881000
Fe	6.675227000	-4.628960000	-2.100827000
O	8.937215000	3.131110000	4.755056000
N	7.958450000	-3.152526000	-1.768546000
N	7.884114000	-5.347666000	-3.509170000
N	5.742293000	-6.381648000	-2.096689000
N	5.848840000	-4.176700000	-0.356054000
C	7.729792000	-2.037771000	-1.003473000
C	8.876557000	-1.171567000	-1.033787000
C	9.804100000	-1.773721000	-1.840150000
C	9.206009000	-2.978726000	-2.329828000
C	9.756810000	-3.779287000	-3.322375000
H	10.732027000	-3.498822000	-3.716123000
C	9.095482000	-4.844771000	-3.919701000
C	9.552798000	-5.536635000	-5.091396000
C	8.582793000	-6.445100000	-5.415266000
C	7.566458000	-6.340421000	-4.406802000
C	6.489278000	-7.209528000	-4.280151000
H	6.340221000	-7.959507000	-5.054501000
C	5.685276000	-7.266820000	-3.148309000
C	4.770461000	-8.333590000	-2.853956000
C	4.305361000	-8.113994000	-1.586990000
C	4.895676000	-6.884655000	-1.138910000
C	4.591567000	-6.253547000	0.059588000
H	3.907636000	-6.756218000	0.740802000
C	5.003311000	-4.969836000	0.391569000
C	4.492958000	-4.233945000	1.506577000

C	4.968466000	-2.956736000	1.388745000
C	5.831499000	-2.937202000	0.242438000
C	6.605187000	-1.831154000	-0.174155000
C	6.267626000	-0.501604000	0.308464000
H	5.853319000	-0.416415000	1.311929000
Cl	4.058646000	-3.101801000	-3.461539000
O	5.542673000	-3.644912000	-3.448746000
O	4.083216000	-1.792482000	-2.793007000
O	3.214673000	-4.068306000	-2.746789000
O	3.714580000	-2.997843000	-4.882496000
H	10.487765000	-5.334534000	-5.606791000
H	8.564901000	-7.148214000	-6.243386000
H	4.541873000	-9.157447000	-3.524341000
H	3.606257000	-8.713751000	-1.010780000
H	3.827233000	-4.634448000	2.265939000
H	4.773105000	-2.125460000	2.056667000
H	10.805771000	-1.430755000	-2.084101000
H	8.986049000	-0.263259000	-0.450881000
H	8.823340000	4.767878000	-2.393441000
H	7.876424000	2.259243000	-2.184572000
H	9.047709000	8.845792000	0.884808000
H	8.111965000	9.289782000	3.398285000
H	4.086994000	7.282929000	6.116184000
H	2.163537000	5.469924000	5.479436000
H	1.845081000	1.565325000	1.957819000
H	3.664465000	0.397324000	0.324615000

Structure [1]**2A•**perchlorate {5/2}

Fe	6.177746000	4.714226000	2.239822000
Cl	8.785312000	3.268512000	3.576031000
N	4.779658000	3.208095000	1.836268000
N	4.757499000	5.575159000	3.516280000
N	6.919588000	6.657564000	2.014634000
N	6.895587000	4.293509000	0.318630000
O	7.322082000	3.916728000	3.605314000
O	8.653159000	1.994452000	2.861389000
O	9.661781000	4.215478000	2.880812000
C	4.976683000	2.128495000	1.023870000
C	3.835265000	1.247617000	1.090887000
C	2.955613000	1.809553000	1.976979000
C	3.564434000	3.018636000	2.456217000
C	3.028314000	3.838560000	3.450562000
H	2.083266000	3.517820000	3.887972000
C	3.596353000	5.005012000	3.969400000
C	3.061591000	5.774039000	5.063518000
C	3.926796000	6.813927000	5.274044000
C	4.966456000	6.692614000	4.284337000
C	5.974464000	7.634859000	4.054660000
H	6.019519000	8.485911000	4.733479000
C	6.849876000	7.645135000	2.965349000
C	7.722493000	8.735694000	2.610499000
C	8.291837000	8.407678000	1.410080000
C	7.788856000	7.104953000	1.055829000
C	8.156609000	6.379364000	-0.080084000
H	8.864245000	6.855970000	-0.757663000
C	7.759194000	5.083515000	-0.409592000
C	8.265047000	4.345289000	-1.531443000
C	7.740303000	3.084545000	-1.446891000
C	6.871618000	3.069653000	-0.296373000
C	6.077456000	1.965980000	0.132945000
C	6.393146000	0.656707000	-0.404227000
H	6.814651000	0.614571000	-1.406876000
Fe	6.473628000	-4.580468000	-2.366784000
O	9.127752000	3.100448000	4.987031000
N	7.871788000	-3.074442000	-1.963102000
N	7.893954000	-5.441481000	-3.643107000
N	5.731790000	-6.523832000	-2.141526000
N	5.755934000	-4.159846000	-0.445471000
C	7.674736000	-1.994800000	-1.150769000
C	8.816162000	-1.113931000	-1.217766000
C	9.695865000	-1.675934000	-2.103768000
C	9.087051000	-2.885017000	-2.583000000
C	9.623211000	-3.704968000	-3.577301000
H	10.568296000	-3.384260000	-4.014655000
C	9.055155000	-4.871396000	-4.096168000
C	9.589912000	-5.640433000	-5.190281000
C	8.724655000	-6.680267000	-5.400859000
C	7.684956000	-6.558905000	-4.411198000
C	6.676890000	-7.501100000	-4.181572000
H	6.631805000	-8.352134000	-4.860412000
C	5.801485000	-7.511381000	-3.092253000
C	4.928935000	-8.601989000	-2.737368000
C	4.359642000	-8.274010000	-1.536916000
C	4.862613000	-6.971278000	-1.182667000
C	4.494954000	-6.245726000	-0.046704000
H	3.787381000	-6.722352000	0.630927000
C	4.892422000	-4.949895000	0.282820000
C	4.386696000	-4.211730000	1.404767000
C	4.911372000	-2.950958000	1.320179000
C	5.779918000	-2.936013000	0.169563000
C	6.573971000	-1.832283000	-0.259824000
C	6.258245000	-0.523019000	0.277307000
H	5.836698000	-0.480884000	1.279941000
Cl	3.866579000	-3.134674000	-3.703384000
O	5.329230000	-3.784186000	-3.732938000
O	4.000010000	-1.860551000	-2.989091000
O	2.989522000	-4.080733000	-3.007662000
O	3.523856000	-2.966677000	-5.114319000
H	10.505103000	-5.410611000	-5.729518000
H	8.795358000	-7.472538000	-6.141393000
H	4.790129000	-9.508496000	-3.320453000
H	3.656887000	-8.856246000	-0.946872000
H	3.707056000	-4.600712000	2.158129000
H	4.736095000	-2.134420000	2.011740000
H	10.679221000	-1.311426000	-2.388580000
H	8.965356000	-0.226693000	-0.611793000
H	8.944811000	4.734217000	-2.284721000
H	7.915662000	2.267977000	-2.138394000
H	8.994646000	8.989883000	0.820068000
H	7.861313000	9.642200000	3.193583000
H	3.856075000	7.606204000	6.014570000
H	2.146433000	5.544174000	5.602792000
H	1.972288000	1.445007000	2.261850000
H	3.686053000	0.360390000	0.484901000

Structure [1]**1•**perchlorate {3/2}

Fe	5.725202000	4.389216000	1.824139000
C	4.231356000	2.159397000	0.478368000
C	2.898889000	1.588970000	0.342635000
C	2.087518000	2.302861000	1.212734000
C	2.934471000	3.255649000	1.878568000
C	2.567136000	3.974746000	3.009240000
H	1.564788000	3.815442000	3.394888000
C	3.413534000	4.799677000	3.737446000
C	3.098382000	5.393040000	5.017488000
C	4.226462000	6.092514000	5.405770000
C	5.178207000	5.952437000	4.326625000
C	6.376844000	6.648222000	4.233919000
H	6.671861000	7.265843000	5.075715000
C	7.147671000	6.712233000	3.080417000
C	8.203556000	7.671194000	2.849616000
C	8.574689000	7.526385000	1.525078000
C	7.790641000	6.429448000	1.004233000
C	7.954916000	5.862330000	-0.251448000
H	8.672035000	6.326846000	-0.920863000
C	7.393714000	4.656504000	-0.657212000
C	7.828171000	3.920834000	-1.813301000
C	7.225773000	2.675469000	-1.745372000
C	6.351789000	2.712064000	-0.582087000
C	5.396423000	1.741009000	-0.210680000
C	2.396863000	0.615745000	-0.690989000
H	1.548743000	0.056286000	-0.269274000
H	3.138589000	-0.141738000	-0.954134000
C	1.946294000	1.295391000	-1.993433000
H	1.639166000	0.533473000	-2.722461000
H	2.764951000	1.873390000	-2.440776000
H	1.104073000	1.978775000	-1.827618000
C	0.612793000	2.153527000	1.448595000
H	0.427458000	2.062239000	2.531782000
H	0.271481000	1.203677000	1.015452000
C	-0.252317000	3.293608000	0.891768000
H	-1.313393000	3.113675000	1.117269000
H	-0.148389000	3.376961000	-0.197455000
H	0.026886000	4.263278000	1.324253000
C	1.796566000	5.243450000	5.748619000

H	1.965360000	5.420791000	6.820574000
H	1.451252000	4.200283000	5.676125000
C	0.679048000	6.178782000	5.263148000
H	-0.242755000	6.006209000	5.837333000
H	0.450522000	6.021000000	4.200757000
H	0.961149000	7.232650000	5.385412000
C	4.456076000	6.871478000	6.667649000
H	5.501344000	6.744395000	6.988264000
H	3.850115000	6.431225000	7.473175000
C	4.134350000	8.370108000	6.570076000
H	4.340789000	8.870032000	7.527526000
H	3.077615000	8.536053000	6.323713000
H	4.734536000	8.863233000	5.793948000
C	8.750441000	8.620696000	3.873570000
H	7.921503000	9.067354000	4.444717000
H	9.240683000	9.461873000	3.362433000
C	9.747302000	7.978285000	4.850616000
H	10.087877000	8.716381000	5.591158000
H	10.629184000	7.595387000	4.321296000
H	9.299848000	7.131934000	5.387563000
C	9.603868000	8.302926000	0.757062000
H	9.659349000	9.323333000	1.164645000
H	9.269822000	8.424589000	-0.284833000
C	11.010942000	7.687391000	0.768651000
H	11.699616000	8.293686000	0.162437000
H	11.007591000	6.666664000	0.365578000
H	11.413780000	7.634369000	1.787898000
C	8.802622000	4.410966000	-2.845650000
H	8.688726000	5.497310000	-2.978421000
H	8.547945000	3.973540000	-3.821101000
C	10.269452000	4.088526000	-2.521715000
H	10.932154000	4.478419000	-3.308063000
H	10.431197000	3.004882000	-2.448117000
H	10.576548000	4.529357000	-1.564573000
C	7.355592000	1.633863000	-2.823464000
H	7.343251000	0.617757000	-2.418150000
H	8.349245000	1.742295000	-3.280563000
C	6.293614000	1.753602000	-3.926497000
H	6.450012000	0.979413000	-4.689743000
H	6.335568000	2.736927000	-4.414596000
H	5.281471000	1.618693000	-3.529005000
C	5.622252000	0.259707000	-0.423725000
H	5.684606000	-0.038292000	-1.475758000
H	4.780123000	-0.289793000	-0.000190000
N	4.205383000	3.223730000	1.350696000
N	4.680772000	5.141668000	3.336405000
N	6.924045000	5.951654000	1.956694000
N	6.464296000	3.936034000	0.050899000
N	8.317774000	-3.176025000	-1.445357000
N	7.842267000	-5.093603000	-3.431319000
N	5.598799000	-5.903434000	-2.051816000
N	6.058770000	-3.888216000	-0.145756000
C	8.291850000	-2.111777000	-0.572935000
C	9.624342000	-1.541485000	-0.437044000
C	10.435724000	-2.255377000	-1.307126000
C	9.588735000	-3.207997000	-1.973149000
C	9.956044000	-3.927003000	-3.103887000
H	10.958411000	-3.767727000	-3.489500000
C	9.109587000	-4.751775000	-3.832218000
C	9.424723000	-5.345040000	-5.112314000
C	8.296537000	-6.044248000	-5.500771000
C	7.344736000	-5.904140000	-4.421680000
C	6.145940000	-6.599683000	-4.329152000
H	5.850825000	-7.217077000	-5.171082000
C	5.375023000	-6.663729000	-3.175708000
C	4.318950000	-7.622524000	-2.945110000
C	3.947869000	-7.477945000	-1.620526000
C	4.732144000	-6.381292000	-1.099439000
C	4.568052000	-5.814458000	0.156403000
H	3.850956000	-6.279053000	0.825788000
C	5.129446000	-4.608797000	0.562384000
C	4.695301000	-3.873357000	1.718745000
C	5.297708000	-2.627995000	1.650924000
C	6.171427000	-2.664390000	0.487439000
C	7.126787000	-1.693317000	0.116064000
C	10.126241000	-0.568229000	0.596612000
H	10.972894000	-0.007044000	0.174214000
H	9.383574000	0.187749000	0.861321000
C	10.579485000	-1.248008000	1.898062000
H	10.886242000	-0.486025000	2.627185000
H	9.762254000	-1.827584000	2.345998000
H	11.422613000	-1.929924000	1.730879000
C	11.910454000	-2.105950000	-1.542920000
H	12.095707000	-2.013689000	-2.626046000
H	12.251802000	-1.156498000	-1.108936000
C	12.775597000	-3.246537000	-0.987180000
H	13.836670000	-3.066324000	-1.212473000
H	12.671641000	-3.330968000	0.101957000
H	12.496482000	-4.215811000	-1.420596000
C	10.726636000	-5.195658000	-5.843311000
H	10.557914000	-5.372918000	-6.915290000
H	11.072156000	-4.152564000	-5.770737000
C	11.843915000	-6.131245000	-5.357780000
H	12.765809000	-5.958833000	-5.931868000
H	12.072372000	-5.973568000	-4.295360000
H	11.561607000	-7.185048000	-5.480126000
C	8.066869000	-6.822996000	-6.762775000
H	7.021660000	-6.695633000	-7.083472000
H	8.673004000	-6.382772000	-7.568186000
C	8.388250000	-8.321709000	-6.665367000
H	8.181794000	-8.821463000	-7.622902000
H	9.444924000	-8.487921000	-6.418919000
H	7.787877000	-8.814801000	-5.889362000
C	3.771857000	-8.571692000	-3.969261000
H	4.600699000	-9.018388000	-4.540517000
H	3.281459000	-9.412885000	-3.458297000
C	2.775113000	-7.928876000	-4.946155000
H	2.434379000	-8.666748000	-5.686848000
H	1.893316000	-7.545911000	-4.416743000
H	3.222729000	-7.082498000	-5.482926000
C	2.918545000	-8.254455000	-0.852671000
H	2.862868000	-9.274766000	-1.260467000
H	3.252572000	-8.376400000	0.189196000
C	1.511594000	-7.638637000	-0.864107000
H	0.822805000	-8.244925000	-0.258018000
H	1.515165000	-6.618001000	-0.460799000
H	1.108749000	-7.585301000	-1.883334000
C	3.721210000	-4.363740000	2.751316000
H	3.835089000	-5.450133000	2.883697000
H	3.976316000	-3.926636000	3.726802000
C	2.254270000	-4.041081000	2.428104000
H	1.591872000	-4.431185000	3.214603000
H	2.092586000	-2.957397000	2.354946000
H	1.946718000	-4.481563000	1.470947000
C	5.168366000	-1.586552000	2.729221000
H	5.180117000	-0.570411000	2.323952000
H	4.175075000	-1.695297000	3.187030000
C	6.231166000	-1.706128000	3.831475000
H	6.075307000	-0.931884000	4.594775000
H	6.189588000	-2.689415000	4.319687000
H	7.243027000	-1.571265000	3.433235000
C	6.900954000	-0.212003000	0.329109000
H	6.838595000	0.085909000	1.381166000
H	7.743092000	0.337504000	-0.094420000
O	5.801161000	-2.897765000	-3.058226000
O	3.434336000	-3.151246000	-2.426944000
Cl	4.320857000	-2.756597000	-3.534611000
O	4.163657000	-1.331041000	-3.872214000
O	4.141440000	-3.617853000	-4.712493000
O	6.722364000	2.945971000	2.963252000
O	9.089040000	3.201236000	2.331948000
Cl	8.202794000	2.805257000	3.439349000
O	8.381808000	3.665668000	4.617914000
O	8.360764000	1.379495000	3.775785000
Fe	6.797824000	-4.341198000	-1.919067000

Structure [1]**1**•perchlorate {5/2}

Fe	5.903662000	4.261351000	2.106644000
C	4.248015000	2.100628000	0.646119000
C	2.921071000	1.485112000	0.587249000
C	2.147442000	2.159973000	1.520944000
C	3.000426000	3.150480000	2.132486000
C	2.646158000	3.924214000	3.240217000
H	1.657011000	3.741634000	3.651555000
C	3.429382000	4.867379000	3.906151000
C	3.048425000	5.578068000	5.112524000
C	4.122873000	6.386050000	5.439861000
C	5.117285000	6.173699000	4.405321000

C	6.308863000	6.890930000	4.270767000
H	6.537747000	7.612102000	5.050401000
C	7.173398000	6.855570000	3.175048000
C	8.258683000	7.785698000	2.937215000
C	8.731735000	7.511944000	1.665387000
C	7.956345000	6.389093000	1.176288000
C	8.139427000	5.754627000	-0.052160000
H	8.905559000	6.172766000	-0.699101000
C	7.521557000	4.587849000	-0.509207000
C	7.915060000	3.876908000	-1.701063000
C	7.228792000	2.673556000	-1.696860000
C	6.364535000	2.705295000	-0.517281000
C	5.392592000	1.743094000	-0.127035000
C	2.366773000	0.513123000	-0.421438000
H	1.429484000	0.098412000	-0.024691000
H	3.014853000	-0.355134000	-0.579983000
C	2.075971000	1.149470000	-1.789002000
H	1.691482000	0.389222000	-2.482473000
H	2.983286000	1.575573000	-2.232981000
H	1.334073000	1.954644000	-1.707794000
C	0.696586000	1.958903000	1.851339000
H	0.571011000	1.968050000	2.946129000
H	0.383347000	0.953863000	1.535752000
C	-0.254432000	2.993642000	1.232744000
H	-1.291523000	2.793225000	1.538702000
H	-0.214497000	2.964721000	0.136432000
H	0.001235000	4.014605000	1.545973000
C	1.739531000	5.435744000	5.832696000
H	1.874269000	5.724436000	6.885203000
H	1.446303000	4.374429000	5.856855000
C	0.589257000	6.261275000	5.237258000
H	-0.336983000	6.097087000	5.806836000
H	0.395776000	5.990861000	4.190762000
H	0.815847000	7.335100000	5.262285000
C	4.267800000	7.320972000	6.605023000
H	5.302024000	7.276952000	6.980478000
H	3.642334000	6.961453000	7.435211000
C	3.901670000	8.782703000	6.307417000
H	4.053181000	9.406117000	7.200578000
H	2.850791000	8.876247000	6.004400000
H	4.515971000	9.196501000	5.496685000
C	8.739087000	8.824668000	3.906455000
H	7.874357000	9.334429000	4.360371000
H	9.285706000	9.606675000	3.359931000
C	9.639715000	8.271840000	5.021425000
H	9.943151000	9.077803000	5.705223000
H	10.548447000	7.816357000	4.607310000
H	9.127486000	7.498544000	5.608616000
C	9.838417000	8.198615000	0.920195000
H	9.918056000	9.238575000	1.269731000
H	9.574558000	8.270032000	-0.146409000
C	11.211207000	7.523119000	1.056573000
H	11.965870000	8.064362000	0.467559000
H	11.185515000	6.482971000	0.706592000
H	11.543954000	7.508102000	2.102331000
C	8.912491000	4.358897000	-2.715736000
H	8.863752000	5.455632000	-2.790167000
H	8.627151000	3.991125000	-3.711503000
C	10.358981000	3.933555000	-2.421854000
H	11.040233000	4.324940000	-3.191460000
H	10.455889000	2.839705000	-2.407934000
H	10.697719000	4.303987000	-1.445247000
C	7.291714000	1.686533000	-2.831657000
H	7.269129000	0.650632000	-2.479017000
H	8.270404000	1.792269000	-3.319986000
C	6.196369000	1.888907000	-3.888389000
H	6.308440000	1.155113000	-4.698051000
H	6.245938000	2.896664000	-4.323170000
H	5.194401000	1.758129000	-3.463904000
C	5.616214000	0.273176000	-0.407774000
H	5.673108000	0.022314000	-1.472583000
H	4.783309000	-0.299956000	-0.002253000
N	4.240550000	3.137609000	1.543439000
N	4.686224000	5.235147000	3.505838000
N	7.031651000	5.999199000	2.110928000
N	6.554381000	3.886079000	0.162690000
N	8.282805000	-3.089698000	-1.638534000
N	7.837029000	-5.187488000	-3.600766000
N	5.491198000	-5.950975000	-2.206193000
N	5.968799000	-3.837957000	-0.257901000
C	8.275399000	-2.052623000	-0.741306000
C	9.602325000	-1.437011000	-0.682702000
C	10.375857000	-2.111932000	-1.616423000
C	9.522856000	-3.102597000	-2.227703000
C	9.877165000	-3.876629000	-3.335212000
H	10.866334000	-3.694171000	-3.746544000
C	9.094010000	-4.820013000	-4.000904000
C	9.475217000	-5.531223000	-5.206899000
C	8.400767000	-6.339200000	-5.534208000
C	7.406075000	-6.126283000	-4.500043000
C	6.214253000	-6.843148000	-4.365739000
H	5.985398000	-7.564371000	-5.145334000
C	5.349416000	-6.807370000	-3.270276000
C	4.263780000	-7.737148000	-3.032630000
C	3.790528000	-7.463151000	-1.760934000
C	4.566199000	-6.340542000	-1.271724000
C	4.383267000	-5.706136000	-0.043231000
H	3.616966000	-6.124085000	0.603631000
C	5.001564000	-4.539667000	0.414012000
C	4.608434000	-3.828921000	1.606090000
C	5.294951000	-2.625707000	1.602040000
C	6.158988000	-2.657361000	0.422305000
C	7.130941000	-1.695157000	0.032040000
C	10.156797000	-0.464851000	0.325732000
H	11.094205000	-0.050520000	-0.071126000
H	9.508942000	0.403645000	0.483958000
C	10.447459000	-1.100829000	1.693489000
H	10.832227000	-0.340479000	2.386691000
H	9.540057000	-1.526516000	2.137675000
H	11.189111000	-1.906252000	1.612480000
C	11.826660000	-1.910855000	-1.947050000
H	11.952124000	-1.920436000	-3.041846000
H	12.139845000	-0.905651000	-1.631922000
C	12.777839000	-2.945238000	-1.328108000
H	13.814885000	-2.744836000	-1.634230000
H	12.737986000	-2.915865000	-0.231805000
H	12.522257000	-3.966359000	-1.640893000
C	10.784343000	-5.389386000	-5.926745000
H	10.649857000	-5.678428000	-6.979188000
H	11.077769000	-4.328133000	-5.951210000
C	11.934304000	-6.214891000	-5.330669000
H	12.860743000	-6.051053000	-5.900027000
H	12.127509000	-5.944124000	-4.284214000
H	11.707556000	-7.288690000	-5.355382000
C	8.256068000	-7.274656000	-6.698968000
H	7.222055000	-7.230430000	-7.074989000
H	8.882107000	-6.915823000	-7.529018000
C	8.621484000	-8.736369000	-6.400394000
H	8.470160000	-9.360212000	-7.293288000
H	9.672187000	-8.830145000	-6.096832000
H	8.006650000	-9.149488000	-5.589723000
C	3.783270000	-8.776026000	-4.001911000
H	4.647940000	-9.285974000	-4.455726000
H	3.236434000	-9.557921000	-3.455439000
C	2.882884000	-8.223027000	-5.116989000
H	2.579334000	-9.028942000	-5.800794000
H	1.974215000	-7.767319000	-4.702982000
H	3.395360000	-7.449870000	-5.704152000
C	2.683434000	-8.149384000	-1.015954000
H	2.603328000	-9.189259000	-1.365634000
H	2.947135000	-8.221064000	0.050673000
C	1.310984000	-7.473215000	-1.152415000
H	0.555993000	-8.014174000	-0.563563000
H	1.337119000	-6.433120000	-0.802308000
H	0.978378000	-7.457914000	-2.198215000
C	3.611113000	-4.310956000	2.620852000
H	3.659551000	-5.407730000	2.694895000
H	3.896831000	-3.943616000	3.616674000
C	2.164676000	-3.885091000	2.327482000
H	1.483504000	-4.276527000	3.097135000
H	2.068077000	-2.791209000	2.313936000
H	1.825580000	-4.255114000	1.350842000
C	5.232354000	-1.638918000	2.737060000
H	5.254731000	-0.602942000	2.384610000
H	4.253824000	-1.744826000	3.225668000
C	6.328003000	-1.841414000	3.793446000
H	6.216149000	-1.107729000	4.603233000
H	6.278555000	-2.849232000	4.228103000
H	7.329854000	-1.710584000	3.368705000
C	6.907305000	-0.225281000	0.312980000

H	6.850404000	0.025348000	1.377833000
H	7.740216000	0.347924000	-0.092402000
O	5.683051000	-2.812077000	-3.269194000
O	3.277660000	-2.928576000	-2.753539000
Cl	4.215990000	-2.711273000	-3.863010000
O	4.136314000	-1.349623000	-4.402010000
O	4.098740000	-3.738512000	-4.902914000
O	6.840385000	2.860197000	3.173585000
O	9.246014000	2.977793000	2.659417000
Cl	8.307073000	2.759901000	3.768269000
O	8.423261000	3.786989000	4.808445000
O	8.387019000	1.398167000	4.307087000
Fe	6.619499000	-4.213244000	-2.201830000

Structure[1]**2**•perchlorate {3/2}

Fe	5.796483000	4.466804000	1.945028000
C	4.436410000	2.135907000	0.633710000
C	3.173130000	1.414003000	0.610473000
C	2.283910000	2.170968000	1.354719000
C	3.033428000	3.276035000	1.892388000
C	2.556840000	4.116504000	2.890911000
H	1.525116000	3.981607000	3.199939000
C	3.329635000	5.014169000	3.614673000
C	2.891064000	5.709338000	4.804719000
C	4.001497000	6.372153000	5.293559000
C	5.069451000	6.117409000	4.352505000
C	6.321575000	6.716648000	4.395338000
H	6.563730000	7.326451000	5.259638000
C	7.222081000	6.701601000	3.337974000
C	8.372199000	7.568353000	3.227785000
C	8.842530000	7.422804000	1.934850000
C	8.016235000	6.411652000	1.316728000
C	8.201400000	5.901502000	0.038878000
H	8.968496000	6.357571000	-0.579152000
C	7.579878000	4.761347000	-0.455643000
C	7.973268000	4.090645000	-1.666405000
C	7.334954000	2.862725000	-1.664428000
C	6.497237000	2.843763000	-0.476399000
C	5.592242000	1.821628000	-0.112637000
C	2.815362000	0.179891000	-0.165870000
H	2.056533000	-0.379235000	0.402026000
H	3.672675000	-0.496000000	-0.238158000
C	2.269257000	0.457235000	-1.573435000
H	2.069111000	-0.488647000	-2.091882000
H	2.988681000	1.018645000	-2.181770000
H	1.339124000	1.038424000	-1.534942000
C	0.823828000	1.921022000	1.596138000
H	0.612327000	1.992141000	2.675637000
H	0.583839000	0.885524000	1.319775000
C	-0.119710000	2.866757000	0.838190000
H	-1.167885000	2.627615000	1.068787000
H	0.016720000	2.777861000	-0.247156000
H	0.055428000	3.916903000	1.106772000
C	1.501701000	5.676479000	5.369545000
H	1.541110000	5.941360000	6.435757000
H	1.113583000	4.646209000	5.339045000
C	0.507825000	6.609882000	4.662587000
H	-0.488239000	6.530160000	5.121512000
H	0.410594000	6.364448000	3.596671000
H	0.829215000	7.657522000	4.730692000
C	4.115446000	7.218220000	6.527586000
H	5.098217000	7.051537000	6.994586000
H	3.380247000	6.870233000	7.267991000
C	3.912550000	8.723208000	6.298349000
H	4.026293000	9.273653000	7.243481000
H	2.910395000	8.934587000	5.903128000
H	4.641100000	9.125031000	5.581692000
C	8.909775000	8.434429000	4.327316000
H	8.080261000	8.963002000	4.823451000
H	9.541961000	9.222539000	3.893812000
C	9.719462000	7.663076000	5.380909000
H	10.065129000	8.343046000	6.172940000
H	10.600520000	7.187277000	4.931349000
H	9.123816000	6.866345000	5.844596000
C	9.997635000	8.122955000	1.281685000
H	10.117884000	9.116817000	1.737750000
H	9.760593000	8.316021000	0.224002000
C	11.332631000	7.369359000	1.371868000
H	12.124823000	7.928968000	0.853595000
H	11.263603000	6.372396000	0.917793000
H	11.641585000	7.231828000	2.415862000
C	8.930543000	4.626208000	-2.692204000
H	8.853510000	5.723035000	-2.733746000
H	8.622252000	4.276714000	-3.687879000
C	10.394913000	4.227071000	-2.456233000
H	11.041486000	4.658539000	-3.234166000
H	10.517803000	3.136283000	-2.480431000
H	10.756246000	4.575413000	-1.479776000
C	7.378058000	1.874017000	-2.794614000
H	7.342481000	0.845254000	-2.421855000
H	8.348942000	1.965916000	-3.301670000
C	6.259403000	2.080149000	-3.826804000
H	6.323102000	1.317534000	-4.614469000
H	6.324784000	3.072011000	-4.295002000
H	5.267674000	1.995533000	-3.366202000
C	5.899297000	0.408401000	-0.481160000
H	5.522977000	-0.017420000	-1.413687000
N	4.316208000	3.277177000	1.399745000
N	4.647972000	5.282688000	3.346995000
N	7.043082000	5.976821000	2.182970000
N	6.631889000	4.026803000	0.216621000
N	8.245162000	-3.215801000	-1.577629000
N	7.909966000	-5.214297000	-3.529629000
N	5.538132000	-5.941699000	-2.337048000
N	5.943874000	-3.983878000	-0.376433000
C	8.126672000	-2.081431000	-0.801537000
C	9.388232000	-1.356704000	-0.778390000
C	10.274919000	-2.104404000	-1.534873000
C	9.525027000	-3.206447000	-2.078363000
C	9.996649000	-4.034748000	-3.089201000
H	11.024541000	-3.891048000	-3.406952000
C	9.222074000	-4.931466000	-3.812259000
C	9.651650000	-5.613309000	-5.013207000
C	8.541728000	-6.284645000	-5.491561000
C	7.484146000	-6.047734000	-4.534314000
C	6.239959000	-6.664303000	-4.561628000
H	5.993924000	-7.274038000	-5.424874000
C	5.355308000	-6.667449000	-3.490873000
C	4.221050000	-7.553206000	-3.366579000
C	3.763605000	-7.414512000	-2.068321000
C	4.580824000	-6.389734000	-1.460406000
C	4.397229000	-5.876676000	-0.183588000
H	3.640336000	-6.340391000	0.441244000
C	5.005244000	-4.725260000	0.301437000
C	4.608382000	-4.053946000	1.510537000
C	5.236523000	-2.820812000	1.503995000
C	6.072077000	-2.798320000	0.314558000
C	6.972822000	-1.773035000	-0.049576000
C	9.746475000	-0.128857000	0.007781000
H	10.516070000	0.426879000	-0.548558000
H	8.893296000	0.553174000	0.072311000
C	10.274082000	-0.415543000	1.420648000
H	10.477650000	0.526846000	1.944486000
H	9.543075000	-0.972123000	2.019556000
H	11.199180000	-1.005331000	1.390592000
C	11.733030000	-1.849118000	-1.782467000
H	11.938979000	-1.912625000	-2.863488000
H	11.972185000	-0.814857000	-1.500734000
C	12.682470000	-2.797520000	-1.035447000
H	13.728981000	-2.555126000	-1.270185000
H	12.551641000	-2.715253000	0.051143000
H	12.507619000	-3.846333000	-1.309434000
C	11.032393000	-5.560418000	-5.597388000
H	10.980435000	-5.816349000	-6.665269000
H	11.409428000	-4.526168000	-5.563253000
C	12.046971000	-6.488797000	-4.913606000
H	13.035403000	-6.392798000	-5.385727000
H	12.156593000	-6.252652000	-3.846797000
H	11.737141000	-7.539512000	-4.987535000
C	8.420091000	-7.123846000	-6.729559000
H	7.428548000	-6.966325000	-7.180897000
H	9.139898000	-6.761582000	-7.478220000
C	8.645007000	-8.627661000	-6.513629000
H	8.523915000	-9.173249000	-7.460664000
H	9.655449000	-8.829255000	-6.134765000
H	7.932245000	-9.043183000	-5.788937000
C	3.686210000	-8.431417000	-4.457871000

H	4.519433000	-8.945526000	-4.962874000
H	3.074788000	-9.230363000	-4.014461000
C	2.848204000	-7.679872000	-5.503550000
H	2.504576000	-8.370016000	-6.287633000
H	1.964462000	-7.218448000	-5.044404000
H	3.422141000	-6.874432000	-5.979467000
C	2.627490000	-8.132242000	-1.401112000
H	2.518661000	-9.128924000	-1.853899000
H	2.879460000	-8.319085000	-0.345769000
C	1.279405000	-7.400819000	-1.478057000
H	0.502365000	-7.971791000	-0.949347000
H	1.337367000	-6.401598000	-1.027489000
H	0.956473000	-7.271228000	-2.518811000
C	3.655222000	-4.592386000	2.538579000
H	3.741800000	-5.688220000	2.586870000
H	3.958909000	-4.234043000	3.532405000
C	2.187697000	-4.207495000	2.298161000
H	1.543890000	-4.639819000	3.077914000
H	2.055354000	-3.117686000	2.315543000
H	1.830812000	-4.564756000	1.323331000
C	5.187259000	-1.830845000	2.632815000
H	5.231162000	-0.802467000	2.260273000
H	4.211436000	-1.917985000	3.131306000
C	6.296248000	-2.041756000	3.674517000
H	6.230801000	-1.277131000	4.459907000
H	6.221912000	-3.032370000	4.143955000
H	7.292000000	-1.963529000	3.221433000
C	6.666908000	-0.360741000	0.324120000
H	7.053973000	0.060544000	1.254216000
O	5.901862000	-2.930120000	-3.277915000
O	3.470245000	-3.180074000	-2.974097000
Cl	4.496461000	-2.733258000	-3.931453000
O	4.400474000	-1.287575000	-4.195258000
O	4.464751000	-3.520368000	-5.173114000
O	6.638138000	2.951120000	3.087599000
O	9.082304000	3.194858000	2.913299000
Cl	8.005929000	2.756232000	3.817752000
O	7.974470000	3.549539000	5.055473000
O	8.081223000	1.311658000	4.092993000
Fe	6.769112000	-4.416243000	-2.110781000

Structure [1]**2**•perchlorate {5/2}

Fe	6.015306000	4.357920000	2.201511000
C	4.491945000	2.114503000	0.732685000
C	3.225312000	1.388488000	0.724617000
C	2.382745000	2.077363000	1.581778000
C	3.151478000	3.171761000	2.128853000
C	2.712961000	3.999829000	3.164032000
H	1.708909000	3.809088000	3.532648000
C	3.433980000	4.996303000	3.823303000
C	2.963436000	5.753028000	4.968570000
C	4.010274000	6.575958000	5.343889000
C	5.080007000	6.326597000	4.396565000
C	6.288209000	7.025277000	4.342454000
H	6.462851000	7.760694000	5.122885000
C	7.238885000	6.954044000	3.322189000
C	8.355631000	7.861633000	3.156114000
C	8.913119000	7.567295000	1.923249000
C	8.150983000	6.457536000	1.387091000
C	8.385953000	5.831567000	0.162414000
H	9.181501000	6.249286000	-0.448366000
C	7.768270000	4.682694000	-0.334982000
C	8.164908000	4.000543000	-1.544498000
C	7.463284000	2.807977000	-1.577768000
C	6.601355000	2.812535000	-0.400056000
C	5.642475000	1.825278000	-0.048308000
C	2.825650000	0.226121000	-0.137235000
H	2.001745000	-0.310571000	0.354932000
H	3.640382000	-0.502204000	-0.208360000
C	2.373396000	0.619236000	-1.551289000
H	2.129160000	-0.278864000	-2.133385000
H	3.159522000	1.160697000	-2.091772000
H	1.486892000	1.266029000	-1.522768000
C	0.945677000	1.788453000	1.904986000
H	0.796443000	1.854561000	2.994893000
H	0.715015000	0.746337000	1.644062000
C	-0.064933000	2.709175000	1.205231000
H	-1.091277000	2.448351000	1.501537000
H	0.005268000	2.618425000	0.113827000
H	0.104377000	3.763845000	1.459709000
C	1.604742000	5.634421000	5.594446000
H	1.654697000	5.989194000	6.633927000
H	1.321815000	4.572055000	5.662208000
C	0.495699000	6.404052000	4.861652000
H	-0.469964000	6.262504000	5.368294000
H	0.385900000	6.065793000	3.822730000
H	0.709664000	7.480544000	4.835798000
C	4.066903000	7.555520000	6.479348000
H	5.070117000	7.531372000	6.932311000
H	3.382322000	7.225772000	7.274541000
C	3.720975000	9.002109000	6.096211000
H	3.801870000	9.661792000	6.972344000
H	2.696083000	9.077279000	5.710242000
H	4.394478000	9.386383000	5.318580000
C	8.786205000	8.898948000	4.150139000
H	7.900657000	9.415070000	4.553491000
H	9.368337000	9.677237000	3.635675000
C	9.617165000	8.340825000	5.315344000
H	9.887108000	9.145384000	6.014683000
H	10.544762000	7.878488000	4.954109000
H	9.066122000	7.572310000	5.873236000
C	10.085304000	8.223403000	1.255170000
H	10.178697000	9.256272000	1.621401000
H	9.890119000	8.314019000	0.175194000
C	11.423026000	7.498620000	1.466928000
H	12.230798000	8.019277000	0.932387000
H	11.382870000	6.463812000	1.102627000
H	11.689730000	7.460508000	2.530893000
C	9.168207000	4.501933000	-2.543553000
H	9.120051000	5.600073000	-2.596617000
H	8.886238000	4.151819000	-3.546736000
C	10.613715000	4.070306000	-2.254652000
H	11.297380000	4.481088000	-3.011865000
H	10.710634000	2.976623000	-2.268647000
H	10.949796000	4.416307000	-1.268162000
C	7.484143000	1.832999000	-2.720597000
H	7.409089000	0.802781000	-2.357548000
H	8.462944000	1.893785000	-3.216949000
C	6.384929000	2.086847000	-3.762953000
H	6.428879000	1.328819000	-4.557105000
H	6.492853000	3.078661000	-4.223328000
H	5.384918000	2.039025000	-3.314506000
C	5.906283000	0.411305000	-0.450498000
H	5.520754000	0.015778000	-1.392903000
N	4.402933000	3.202560000	1.566507000
N	4.713882000	5.358652000	3.498525000
N	7.159588000	6.087967000	2.259668000
N	6.786884000	3.972706000	0.310601000
N	8.161862000	-3.157530000	-1.706620000
N	7.854551000	-5.272118000	-3.681528000
N	5.421772000	-6.043218000	-2.445411000
N	5.782264000	-3.957549000	-0.463739000
C	8.070092000	-2.086401000	-0.851951000
C	9.337453000	-1.362259000	-0.822266000
C	10.183443000	-2.034817000	-1.689072000
C	9.415529000	-3.115967000	-2.263439000
C	9.854144000	-3.918731000	-3.318247000
H	10.857991000	-3.719095000	-3.682754000
C	9.132317000	-4.898553000	-4.001540000
C	9.599868000	-5.624301000	-5.167839000
C	8.553557000	-6.440298000	-5.559823000
C	7.487447000	-6.218778000	-4.601577000
C	6.283034000	-6.925172000	-4.556298000
H	6.106831000	-7.642276000	-5.353280000
C	5.340434000	-6.885621000	-3.526620000
C	4.232096000	-7.805659000	-3.371560000
C	3.682762000	-7.543180000	-2.127892000
C	4.439257000	-6.437927000	-1.574203000
C	4.202263000	-5.833809000	-0.338789000
H	3.412579000	-6.268748000	0.267572000
C	4.807359000	-4.684193000	0.172732000
C	4.402555000	-4.018386000	1.388930000
C	5.092233000	-2.819118000	1.435573000
C	5.957237000	-2.804178000	0.260492000
C	6.914095000	-1.809554000	-0.073960000

C	9.732977000	-0.217154000	0.064509000
H	10.570484000	0.318620000	-0.404893000
H	8.924593000	0.518702000	0.131835000
C	10.156788000	-0.635320000	1.480258000
H	10.394375000	0.252081000	2.081419000
H	9.358546000	-1.182492000	1.996736000
H	11.040651000	-1.286114000	1.457709000
C	11.623389000	-1.742883000	-1.996249000
H	11.779807000	-1.782173000	-3.086434000
H	11.855842000	-0.708537000	-1.707572000
C	12.625751000	-2.684419000	-1.312547000
H	13.655092000	-2.420678000	-1.595554000
H	12.548383000	-2.619680000	-0.219714000
H	12.453998000	-3.731934000	-1.593635000
C	10.955502000	-5.485000000	-5.796170000
H	10.901322000	-5.808399000	-6.845655000
H	11.236380000	-4.420584000	-5.833159000
C	12.069247000	-6.274174000	-5.091854000
H	13.032098000	-6.116587000	-5.599119000
H	12.184073000	-5.966105000	-4.044101000
H	11.856778000	-7.351238000	-5.096266000
C	8.494695000	-7.389844000	-6.720384000
H	7.489612000	-7.355941000	-7.168587000
H	9.175480000	-7.037826000	-7.509275000
C	8.845150000	-8.845414000	-6.377211000
H	8.759802000	-9.482053000	-7.269810000
H	9.872520000	-8.929094000	-5.999656000
H	8.177004000	-9.250994000	-5.605813000
C	3.801759000	-8.824677000	-4.384452000
H	4.687886000	-9.327678000	-4.802904000
H	3.226502000	-9.616472000	-3.883055000
C	2.961524000	-8.247772000	-5.533750000
H	2.690731000	-9.040014000	-6.246670000
H	2.034233000	-7.796181000	-5.158363000
H	3.505996000	-7.466575000	-6.080380000
C	2.521361000	-8.222965000	-1.464586000
H	2.437135000	-9.250680000	-1.847117000
H	2.723496000	-8.329124000	-0.387330000
C	1.174693000	-7.509504000	-1.657257000
H	0.375829000	-8.046988000	-1.125994000
H	1.206080000	-6.480021000	-1.277395000
H	0.901052000	-7.458027000	-2.718889000
C	3.401825000	-4.539165000	2.380617000
H	3.460221000	-5.637290000	2.422798000
H	3.678164000	-4.196336000	3.387890000
C	1.952984000	-4.118305000	2.092364000
H	1.271315000	-4.543690000	2.843275000
H	1.845487000	-3.025831000	2.117717000
H	1.622985000	-4.456859000	1.101273000
C	5.057437000	-1.852534000	2.585419000
H	5.124469000	-0.819245000	2.228991000
H	4.077085000	-1.926054000	3.076975000
C	6.154085000	-2.101254000	3.631671000
H	6.098689000	-1.347880000	4.429703000
H	6.054013000	-3.096399000	4.086562000
H	7.155683000	-2.041236000	3.188383000
C	6.645700000	-0.399644000	0.339982000
H	7.042895000	-0.010295000	1.279939000
O	5.721070000	-2.875427000	-3.463208000
O	3.282719000	-3.114222000	-3.193659000
Cl	4.308864000	-2.729653000	-4.171659000
O	4.232020000	-1.310105000	-4.532475000
O	4.325939000	-3.613758000	-5.341609000
O	6.832090000	2.930862000	3.318056000
O	9.280524000	3.068701000	3.094314000
Cl	8.220183000	2.803919000	4.076052000
O	8.208180000	3.787622000	5.163613000
O	8.238903000	1.420501000	4.561578000
Fe	6.551540000	-4.305956000	-2.361108000

Structure [11]**1**•picrate

Fe	-0.927001000	17.512361000	6.555261000
Fe	-2.652512000	8.681926000	3.093412000
H	-3.679644000	20.442279000	11.556941000
H	-4.522387000	19.080741000	10.853289000
C	-5.110407000	20.999013000	10.040352000
H	-5.931038000	21.126286000	10.761054000
H	-5.540076000	20.624546000	9.101727000
H	-4.684428000	21.989574000	9.834394000
C	-1.101525000	21.396742000	10.702588000
H	-0.046162000	21.177545000	10.927211000
H	-1.630294000	21.285690000	11.660430000
C	-1.224587000	22.854479000	10.234498000
H	-0.801834000	23.535770000	10.986995000
H	-2.273981000	23.135218000	10.076961000
H	-0.693501000	23.022432000	9.288078000
C	3.035107000	21.543518000	7.165934000
H	2.393706000	22.281242000	7.673960000
H	3.612047000	22.117199000	6.426739000
C	4.005537000	20.931827000	8.187804000
H	4.603532000	21.718987000	8.669123000
H	4.694174000	20.225465000	7.706624000
H	3.471351000	20.383030000	8.974754000
C	3.361812000	20.410612000	4.144596000
H	3.684391000	21.448766000	4.313182000
H	2.903973000	20.409383000	3.143382000
C	4.598911000	19.500446000	4.136106000
H	5.294064000	19.807379000	3.341274000
H	4.327618000	18.450110000	3.969648000
H	5.133839000	19.549091000	5.092871000
C	0.961429000	16.574689000	1.261747000
H	1.127816000	17.646900000	1.079745000
H	0.394994000	16.220304000	0.388826000
C	2.315162000	15.850379000	1.307472000
H	2.883464000	16.036989000	0.384699000
H	2.180437000	14.765227000	1.408611000
H	2.923008000	16.185713000	2.158252000
C	-1.178913000	14.343365000	1.764630000
H	-1.326382000	13.355641000	2.211957000
H	-0.351584000	14.202740000	1.055853000
C	-2.433843000	14.733769000	0.970848000
H	-2.670034000	13.953816000	0.234636000
H	-2.287076000	15.681691000	0.435411000
H	-3.304672000	14.857619000	1.625955000
C	-2.454188000	13.452064000	4.625879000
H	-2.748258000	13.133590000	3.618105000
H	-3.229691000	13.083877000	5.296724000
N	-2.853705000	16.724967000	6.414629000
N	-1.640520000	18.888678000	7.953352000
N	0.500897000	18.971957000	6.116829000
N	-0.749824000	16.820759000	4.592408000
N	-0.725840000	9.469335000	3.233672000
N	-1.939298000	7.305718000	1.695168000
N	-4.080230000	7.222182000	3.532238000
N	-2.829362000	9.373509000	5.056319000
C	-0.367323000	10.588862000	3.941940000
C	1.031700000	10.923894000	3.661733000
C	1.469082000	9.988996000	2.735627000
C	0.348097000	9.125402000	2.452565000
C	0.338342000	8.151784000	1.450969000
H	1.250524000	8.058787000	0.868433000
C	-0.717889000	7.324316000	1.071798000
C	-0.698941000	6.396236000	-0.042454000
C	-1.954507000	5.816642000	-0.085018000
C	-2.697108000	6.377376000	1.027548000
C	-3.967799000	5.967027000	1.439825000
H	-4.466381000	5.224166000	0.822981000
C	-4.590128000	6.309906000	2.643109000
C	-5.761198000	5.657398000	3.196118000
C	-5.905379000	6.148503000	4.481802000
C	-4.851456000	7.128463000	4.662133000
C	-4.654547000	7.901522000	5.805755000
H	-5.333787000	7.714287000	6.632796000
C	-3.741845000	8.943690000	5.986674000
C	-3.712999000	9.800471000	7.146380000
C	-2.814342000	10.818115000	6.870870000
C	-2.265097000	10.526091000	5.548373000
C	-1.240346000	11.239308000	4.862033000
C	1.945208000	11.889772000	4.369176000
H	2.822962000	12.066745000	3.732038000
H	1.496091000	12.877735000	4.508441000
C	2.435379000	11.385550000	5.734719000
H	3.098301000	12.131805000	6.194179000
H	1.598975000	11.209125000	6.421319000
H	2.991206000	10.443753000	5.640665000
C	2.834054000	9.845106000	2.127433000
H	2.728643000	9.681866000	1.042998000
H	3.379318000	10.794157000	2.220843000

C	3.691567000	8.718694000	2.722026000
H	4.663032000	8.665164000	2.209742000
H	3.882159000	8.885080000	3.789835000
H	3.201209000	7.741210000	2.623294000
C	0.467798000	6.152644000	-0.953979000
H	0.098844000	5.752620000	-1.909217000
H	0.941701000	7.114176000	-1.205712000
C	1.530050000	5.195886000	-0.393047000
H	2.350507000	5.068708000	-1.113964000
H	1.959930000	5.570315000	0.545495000
H	1.104180000	4.205287000	-0.187043000
C	-2.479179000	4.798396000	-1.054575000
H	-3.534684000	5.017533000	-1.278573000
H	-1.950920000	4.909936000	-2.012647000
C	-2.355678000	3.340484000	-0.587155000
H	-2.778788000	2.659455000	-1.339688000
H	-1.306166000	3.059791000	-0.430338000
H	-2.886203000	3.172084000	0.359502000
C	-6.614229000	4.650091000	2.483907000
H	-5.972838000	3.912465000	1.975721000
H	-7.190848000	4.076326000	3.223288000
C	-7.585080000	5.261548000	1.462297000
H	-8.183324000	4.474276000	0.981469000
H	-8.273473000	5.968081000	1.943576000
H	-7.051228000	5.810090000	0.674941000
C	-6.940095000	5.782756000	5.505421000
H	-7.262321000	4.744453000	5.337068000
H	-6.481967000	5.784298000	6.506499000
C	-8.177530000	6.692463000	5.514143000
H	-8.872297000	6.385452000	6.309284000
H	-7.906557000	7.742934000	5.680272000
H	-8.712776000	6.643411000	4.557576000
C	-4.540258000	9.619828000	8.387142000
H	-4.706461000	8.547629000	8.569390000
H	-3.973856000	9.974507000	9.259963000
C	-5.894107000	10.343915000	8.341291000
H	-6.462378000	10.157388000	9.264100000
H	-5.759540000	11.429070000	8.239955000
H	-6.501900000	10.008341000	7.490567000
C	-2.400208000	11.851288000	7.883770000
H	-2.252765000	12.838944000	7.436294000
H	-3.227539000	11.992006000	8.592528000
C	-1.145248000	11.461058000	8.677593000
H	-0.909138000	12.241088000	9.413748000
H	-1.291916000	10.513160000	9.213097000
H	-0.274405000	11.337254000	8.022492000
C	-1.125044000	12.742280000	5.022311000
H	-0.830902000	13.060864000	6.030027000
H	-0.349558000	13.110344000	4.351378000
O	0.069536000	16.219224000	7.674805000
C	0.920861000	16.075307000	8.620431000
C	0.547268000	15.994341000	10.010728000
O	-1.610806000	15.245100000	9.711784000
N	-0.869626000	15.943260000	10.393866000
C	2.345732000	16.026514000	8.403420000
N	2.889387000	16.009524000	7.040246000
O	2.283827000	15.353982000	6.200374000
O	3.936383000	16.624113000	6.846379000
C	3.272630000	15.974123000	9.433591000
H	4.336774000	15.968245000	9.210278000
C	2.830675000	15.924124000	10.755070000
C	1.466400000	15.943592000	11.046942000
H	1.125199000	15.915170000	12.079061000
O	-1.201957000	16.575072000	11.393814000
N	3.804541000	15.853361000	11.843525000
O	3.367282000	15.812783000	12.991968000
O	4.995374000	15.842118000	11.537505000
O	-3.649873000	9.974963000	1.974530000
C	-4.501245000	10.118981000	1.028961000
C	-4.127802000	10.200327000	-0.361347000
O	-1.969664000	10.949379000	-0.062336000
N	-2.710964000	10.251575000	-0.744655000
C	-5.926098000	10.167558000	1.246125000
N	-6.469574000	10.183978000	2.609383000
O	-7.516192000	9.568762000	2.803267000
O	-5.864237000	10.839667000	3.449296000
C	-6.853127000	10.220203000	0.216098000
H	-7.917251000	10.225905000	0.439513000
C	-6.411309000	10.270656000	-1.105420000
C	-5.047072000	10.251332000	-1.397440000
H	-4.705984000	10.280069000	-2.429587000
O	-2.378780000	9.620249000	-1.744963000
N	-7.385294000	10.341723000	-2.193748000
O	-6.948163000	10.382641000	-3.342227000
O	-8.576093000	10.352879000	-1.887589000
C	-3.212102000	15.605399000	5.706351000
C	-4.611123000	15.270272000	5.986482000
C	-5.048633000	16.205173000	6.912521000
C	-3.927722000	17.068847000	7.195640000
C	-3.918185000	18.042566000	8.197143000
H	-4.830475000	18.135564000	8.779510000
C	-2.862091000	18.870166000	8.576399000
C	-2.881383000	19.798507000	9.690436000
C	-1.625868000	20.378188000	9.733179000
C	-0.882931000	19.817194000	8.620965000
C	0.387947000	20.227345000	8.209076000
H	0.886390000	20.970254000	8.825975000
C	1.010681000	19.884188000	7.006084000
C	2.182105000	20.536375000	6.453459000
C	2.326649000	20.045143000	5.167861000
C	1.272556000	19.065437000	4.987199000
C	1.075771000	18.292496000	3.843479000
H	1.755263000	18.479643000	3.016626000
C	0.162876000	17.250552000	3.662248000
C	0.134072000	16.393924000	2.502429000
C	-0.764745000	15.376356000	2.777701000
C	-1.314129000	15.668285000	4.100155000
C	-2.338969000	14.955025000	4.786320000
C	-5.524526000	14.304319000	5.279010000
H	-6.402320000	14.127329000	5.916088000
H	-5.075354000	13.316372000	5.139830000
C	-6.014619000	14.808443000	3.913404000
H	-6.677556000	14.062176000	3.453983000
H	-5.178179000	14.984762000	3.226820000
H	-6.570408000	15.750275000	4.007342000
C	-6.413659000	16.348967000	7.520621000
H	-6.308331000	16.512240000	8.605060000
H	-6.958831000	15.399865000	7.427193000
C	-7.271239000	17.475280000	6.925938000
H	-8.242750000	17.528719000	7.438144000
H	-7.461729000	17.308855000	5.858117000
H	-6.780992000	18.452816000	7.024688000
C	-4.048359000	20.042226000	10.601621000

Structure ^{1}**1**•picrate{3/2}

Fe	-1.181216000	17.630360000	6.356901000
Fe	-2.466839000	8.541596000	3.339622000
C	-3.346122000	15.602010000	5.859828000
C	-4.722156000	15.286387000	6.222103000
C	-5.101692000	16.238219000	7.155885000
C	-3.956700000	17.079592000	7.374970000
C	-3.846712000	17.984503000	8.423099000
H	-4.695065000	18.070314000	9.094624000
C	-2.705657000	18.707626000	8.738412000
C	-2.529406000	19.504427000	9.930765000
C	-1.244819000	20.013313000	9.868187000
C	-0.691676000	19.558379000	8.612446000
C	0.508650000	20.001566000	8.069717000
H	1.128033000	20.656862000	8.673852000
C	0.877082000	19.797845000	6.744961000
C	1.914608000	20.533857000	6.057654000
C	1.819526000	20.179814000	4.724347000
C	0.777277000	19.180674000	4.646098000
C	0.449286000	18.463060000	3.505152000
H	0.968204000	18.719793000	2.587203000
C	-0.382944000	17.349787000	3.473704000
C	-0.476775000	16.455510000	2.352894000
C	-1.211979000	15.360285000	2.775079000
C	-1.627777000	15.652793000	4.138736000
C	-2.543036000	14.910726000	4.919357000
C	-5.672173000	14.317248000	5.570239000
H	-6.420533000	14.004962000	6.313312000
H	-5.180957000	13.395073000	5.252986000
C	-6.403212000	14.904746000	4.353400000
H	-7.058507000	14.143289000	3.907950000
H	-5.693398000	15.231904000	3.583172000
H	-7.019143000	15.770142000	4.627621000
C	-6.429986000	16.404545000	7.834562000

H	-6.270948000	16.479433000	8.922828000
H	-7.026496000	15.493408000	7.692565000
C	-7.251942000	17.614414000	7.366688000
H	-8.199353000	17.669858000	7.921799000
H	-7.491051000	17.545530000	6.297797000
H	-6.711862000	18.557357000	7.522669000
C	-3.553682000	19.689112000	11.011189000
H	-3.040004000	19.947418000	11.948178000
H	-4.051914000	18.727745000	11.209350000
C	-4.614377000	20.759848000	10.716054000
H	-5.327587000	20.831379000	11.549750000
H	-5.182423000	20.531010000	9.804425000
H	-4.156118000	21.747772000	10.577871000
C	-0.534853000	20.883592000	10.863121000
H	0.527707000	20.599044000	10.904241000
H	-0.930441000	20.670602000	11.866816000
C	-0.645505000	22.392208000	10.596550000
H	-0.090663000	22.957190000	11.359339000
H	-1.690644000	22.726380000	10.622536000
H	-0.238442000	22.660578000	9.612686000
C	2.865245000	21.501152000	6.698724000
H	2.313255000	22.164496000	7.383443000
H	3.280777000	22.160861000	5.923832000
C	4.023280000	20.840382000	7.461804000
H	4.685277000	21.607083000	7.889156000
H	4.620944000	20.200326000	6.800913000
H	3.661406000	20.208729000	8.283650000
C	2.633379000	20.679668000	3.567021000
H	2.929850000	21.721065000	3.762020000
H	2.001724000	20.723016000	2.666614000
C	3.892143000	19.852935000	3.265093000
H	4.412999000	20.258942000	2.385943000
H	3.647972000	18.801804000	3.065540000
H	4.590592000	19.867870000	4.110983000
C	0.158272000	16.670059000	1.009389000
H	0.188903000	17.745672000	0.780341000
H	-0.480116000	16.228312000	0.231383000
C	1.572932000	16.082623000	0.889057000
H	1.991277000	16.291045000	-0.106217000
H	1.564751000	14.993861000	1.031168000
H	2.250051000	16.505629000	1.642526000
C	-1.626342000	14.242854000	1.857731000
H	-1.643931000	13.271017000	2.358997000
H	-0.858104000	14.136472000	1.080053000
C	-2.978461000	14.486306000	1.171441000
H	-3.190603000	13.674671000	0.463036000
H	-2.979985000	15.434503000	0.616699000
H	-3.800602000	14.525402000	1.896458000
C	-2.635876000	13.400344000	4.832963000
H	-3.000833000	13.030149000	3.867597000
H	-3.351886000	13.054755000	5.578838000
N	-2.937817000	16.743565000	6.513505000
N	-1.576639000	18.736162000	7.955628000
N	0.210141000	18.964654000	5.878415000
N	-1.122623000	16.877392000	4.530786000
N	-0.677353000	9.334106000	3.591789000
N	-1.754185000	7.296993000	1.967996000
N	-4.071277000	7.380516000	3.437118000
N	-2.904498000	9.321782000	5.098912000
C	-0.403057000	10.533556000	4.217080000
C	1.009534000	10.866395000	4.052018000
C	1.565536000	9.826546000	3.323790000
C	0.490644000	8.929823000	2.993158000
C	0.608049000	7.886302000	2.082926000
H	1.593324000	7.698863000	1.668801000
C	-0.449317000	7.154467000	1.563018000
C	-0.347894000	6.223250000	0.461723000
C	-1.641331000	5.835552000	0.164913000
C	-2.491246000	6.486541000	1.137229000
C	-3.850912000	6.242971000	1.288887000
H	-4.341120000	5.615066000	0.551457000
C	-4.574659000	6.604303000	2.420022000
C	-5.867097000	6.063709000	2.776141000
C	-6.100799000	6.453889000	4.082909000
C	-4.981333000	7.284840000	4.461999000
C	-4.840920000	7.930450000	5.682122000
H	-5.594663000	7.739027000	6.439540000
C	-3.881802000	8.894581000	5.968345000
C	-3.887607000	9.703303000	7.155309000
C	-2.965324000	10.716606000	6.949979000
C	-2.370786000	10.468284000	5.646806000
C	-1.339281000	11.217260000	5.026644000
C	1.818539000	11.964022000	4.689231000
H	2.731531000	12.102637000	4.093544000
H	1.314792000	12.933791000	4.654534000
C	2.228324000	11.678065000	6.140966000
H	2.840985000	12.504190000	6.526453000
H	1.353510000	11.576699000	6.793729000
H	2.812588000	10.752397000	6.220194000
C	2.997872000	9.624586000	2.922912000
H	3.039299000	9.348193000	1.857530000
H	3.535438000	10.579685000	2.990731000
C	3.752601000	8.570355000	3.745686000
H	4.785843000	8.470508000	3.383380000
H	3.793017000	8.847131000	4.806998000
H	3.273622000	7.584378000	3.679972000
C	0.927110000	5.809892000	-0.211622000
H	0.694426000	5.428363000	-1.215699000
H	1.558502000	6.696805000	-0.376307000
C	1.733066000	4.747453000	0.549863000
H	2.652183000	4.496941000	0.000933000
H	2.021031000	5.095765000	1.550728000
H	1.152779000	3.824161000	0.677144000
C	-2.114442000	4.910883000	-0.917653000
H	-3.074291000	5.274824000	-1.314830000
H	-1.413764000	4.965287000	-1.763405000
C	-2.266312000	3.443436000	-0.491029000
H	-2.634268000	2.836888000	-1.331063000
H	-1.306778000	3.021408000	-0.165221000
H	-2.973937000	3.335089000	0.341732000
C	-6.739973000	5.230655000	1.885359000
H	-6.141091000	4.436557000	1.411279000
H	-7.483640000	4.707241000	2.502438000
C	-7.472079000	6.030543000	0.797333000
H	-8.121783000	5.368671000	0.207169000
H	-8.094814000	6.820006000	1.237344000
H	-6.768710000	6.516092000	0.108360000
C	-7.276236000	6.126103000	4.956021000
H	-7.672940000	5.141423000	4.667640000
H	-6.938542000	6.007206000	5.996970000
C	-8.414547000	7.156009000	4.906510000
H	-9.221477000	6.866558000	5.595144000
H	-8.065577000	8.158457000	5.185488000
H	-8.839069000	7.231088000	3.897518000
C	-4.765930000	9.489128000	8.354624000
H	-4.963826000	8.414504000	8.482623000
H	-4.222481000	9.792786000	9.260492000
C	-6.099240000	10.249730000	8.296540000
H	-6.699779000	10.040413000	9.193576000
H	-5.935238000	11.334115000	8.244570000
H	-6.689423000	9.964813000	7.415581000
C	-2.545084000	11.690125000	8.016087000
H	-2.243413000	12.656707000	7.605818000
H	-3.414052000	11.912378000	8.651082000
C	-1.413409000	11.151691000	8.904713000
H	-1.154162000	11.893344000	9.672058000
H	-1.705465000	10.220862000	9.409235000
H	-0.511276000	10.937704000	8.318307000
C	-1.271700000	12.727911000	5.156497000
H	-0.918383000	13.077999000	6.135359000
H	-0.547044000	13.096402000	4.429653000
O	0.039927000	16.219902000	7.277651000
C	0.966960000	16.059841000	8.131156000
C	0.726132000	15.838102000	9.543887000
O	-1.402272000	14.979142000	9.345821000
N	-0.640320000	15.647292000	10.036866000
C	2.379087000	16.127255000	7.806518000
N	2.811332000	16.260638000	6.412889000
O	2.190238000	15.631253000	5.563503000
O	3.793882000	16.968439000	6.191794000
C	3.388753000	16.061153000	8.753396000
H	4.428952000	16.146624000	8.448035000
C	3.065628000	15.877673000	10.098777000
C	1.731083000	15.774845000	10.495188000
H	1.480826000	15.637543000	11.544507000
O	-0.920542000	16.139585000	11.128979000
N	4.127102000	15.790843000	11.094269000
O	3.793660000	15.640488000	12.269626000
O	5.288786000	15.876810000	10.696093000
O	-3.241575000	10.015580000	2.085647000

C	-3.956058000	10.174223000	1.046699000
C	-3.422433000	10.153854000	-0.301133000
O	-1.288802000	10.851039000	0.208576000
N	-1.972321000	10.136743000	-0.516939000
C	-5.394597000	10.350163000	1.078718000
N	-6.086313000	10.531810000	2.356014000
O	-7.210234000	10.042207000	2.468051000
O	-5.516904000	11.194249000	3.217436000
C	-6.188766000	10.378293000	-0.057042000
H	-7.267726000	10.476375000	0.035640000
C	-5.597099000	10.289064000	-1.317689000
C	-4.210236000	10.175951000	-1.439766000
H	-3.750156000	10.117274000	-2.423506000
O	-1.546142000	9.441501000	-1.437611000
N	-6.429829000	10.324141000	-2.513682000
O	-5.863918000	10.236176000	-3.603295000
O	-7.645853000	10.434440000	-2.357574000

Structure [7]**1**•picrate

Fe	-1.162764000	17.640515000	6.342533000
Fe	-2.409620000	8.556821000	3.299975000
H	-3.790378000	20.444827000	11.396240000
H	-4.723285000	19.195964000	10.603444000
C	-5.083678000	21.188134000	9.835796000
H	-5.925023000	21.368776000	10.520115000
H	-5.496850000	20.888510000	8.863420000
H	-4.556149000	22.139882000	9.689510000
C	-1.076202000	21.120411000	10.732290000
H	-0.058744000	20.780751000	10.979375000
H	-1.653388000	21.001483000	11.660676000
C	-1.036733000	22.609659000	10.359264000
H	-0.582116000	23.195521000	11.171076000
H	-2.046044000	23.003730000	10.183397000
H	-0.451391000	22.783177000	9.446498000
C	3.106467000	21.142983000	7.288716000
H	2.529276000	21.895763000	7.849181000
H	3.729314000	21.714895000	6.586678000
C	4.022483000	20.382795000	8.259556000
H	4.704311000	21.080273000	8.766760000
H	4.626932000	19.634350000	7.731560000
H	3.448012000	19.851902000	9.029806000
C	3.293863000	20.284709000	4.165682000
H	3.674419000	21.287089000	4.411745000
H	2.819388000	20.390667000	3.178019000
C	4.478869000	19.314100000	4.058135000
H	5.176030000	19.647626000	3.275916000
H	4.147044000	18.297076000	3.813346000
H	5.031620000	19.254921000	5.004051000
C	0.683130000	16.676119000	1.144287000
H	0.823562000	17.752741000	0.966925000
H	0.081365000	16.320286000	0.296076000
C	2.047941000	15.971590000	1.118432000
H	2.567752000	16.174382000	0.170894000
H	1.934505000	14.883781000	1.215998000
H	2.691023000	16.309205000	1.941716000
C	-1.373968000	14.377306000	1.743421000
H	-1.525780000	13.397364000	2.203576000
H	-0.563496000	14.220523000	1.018729000
C	-2.644200000	14.771406000	0.975444000
H	-2.899845000	13.987851000	0.249717000
H	-2.507471000	15.715073000	0.430089000
H	-3.498662000	14.901479000	1.650821000
C	-2.468280000	13.428992000	4.673496000
H	-2.858497000	13.062214000	3.715210000
H	-3.158432000	13.065413000	5.435629000
N	-2.953165000	16.812527000	6.277323000
N	-1.740832000	18.838204000	7.816493000
N	0.376333000	18.860601000	6.066731000
N	-0.898171000	16.870737000	4.543679000
N	-0.623063000	9.395573000	3.329630000
N	-1.857291000	7.370930000	1.806653000
N	-3.929147000	7.319084000	3.609492000
N	-2.641794000	9.322739000	5.105476000
C	-0.284328000	10.574628000	3.959679000
C	1.107346000	10.907390000	3.674056000
C	1.577857000	9.906827000	2.838230000
C	0.470105000	9.026708000	2.582501000
C	0.475867000	8.043865000	1.600349000
H	1.396766000	7.907624000	1.042675000
C	-0.629290000	7.310624000	1.193997000
C	-0.669161000	6.443712000	0.038022000
C	-1.975004000	6.001387000	-0.066812000
C	-2.682166000	6.559169000	1.064367000
C	-3.982639000	6.228249000	1.425912000
H	-4.547956000	5.588705000	0.755504000
C	-4.533710000	6.519103000	2.668573000
C	-5.717657000	5.890670000	3.209775000
C	-5.773936000	6.258721000	4.541995000
C	-4.667965000	7.163927000	4.757436000
C	-4.409458000	7.838012000	5.942267000
H	-5.042973000	7.612554000	6.794350000
C	-3.493611000	8.873430000	6.087115000
C	-3.427371000	9.727013000	7.241298000
C	-2.596455000	10.784003000	6.907680000
C	-2.111514000	10.510679000	5.564253000
C	-1.150323000	11.260277000	4.844977000
C	1.985373000	11.956665000	4.301227000
H	2.767213000	12.232162000	3.578357000
H	1.449928000	12.885621000	4.506593000
C	2.661547000	11.497950000	5.601979000
H	3.282040000	12.309500000	6.005950000
H	1.919548000	11.229131000	6.363921000
H	3.303736000	10.623330000	5.440533000
C	2.956681000	9.734139000	2.270727000
H	2.880139000	9.582001000	1.181824000
H	3.519099000	10.669460000	2.391604000
C	3.770634000	8.583324000	2.880098000
H	4.761146000	8.523820000	2.406645000
H	3.920022000	8.727146000	3.957629000
H	3.271715000	7.614865000	2.744405000
C	0.493549000	6.135479000	-0.858035000
H	0.113742000	5.806435000	-1.835607000
H	1.055053000	7.060537000	-1.060717000
C	1.453963000	5.068110000	-0.312889000
H	2.279299000	4.899099000	-1.019329000
H	1.888796000	5.366788000	0.650232000
H	0.939558000	4.110562000	-0.158162000
C	-2.577777000	5.108132000	-1.110795000
H	-3.607794000	5.435034000	-1.319883000
H	-2.033361000	5.248733000	-2.055902000
C	-2.582412000	3.613651000	-0.757387000
H	-3.056329000	3.031852000	-1.561041000
H	-1.561939000	3.232591000	-0.622122000
H	-3.132851000	3.418979000	0.172710000
C	-6.658137000	5.003135000	2.449660000
H	-6.084368000	4.263086000	1.869127000
H	-7.252027000	4.416955000	3.164969000
C	-7.612427000	5.753690000	1.508741000
H	-8.293129000	5.047516000	1.012135000
H	-8.217935000	6.485619000	2.058223000
H	-7.067446000	6.302469000	0.729608000
C	-6.777941000	5.849876000	5.579494000
H	-7.149771000	4.842557000	5.340352000
H	-6.276901000	5.748634000	6.554444000
C	-7.974076000	6.802488000	5.719831000
H	-8.644332000	6.458953000	6.521031000
H	-7.650845000	7.824433000	5.955352000
H	-8.553870000	6.853098000	4.789718000
C	-4.171984000	9.516103000	8.528222000
H	-4.296447000	8.438894000	8.713693000
H	-3.561917000	9.883924000	9.365289000
C	-5.544905000	10.204047000	8.571084000
H	-6.047342000	10.000695000	9.527826000
H	-5.446563000	11.292573000	8.465299000
H	-6.196414000	9.853526000	7.759936000
C	-2.158316000	11.838629000	7.886115000
H	-2.030003000	12.818380000	7.418504000
H	-2.961782000	11.985917000	8.620444000
C	-0.871839000	11.471553000	8.640171000
H	-0.622788000	12.262615000	9.360071000
H	-0.984405000	10.527645000	9.190588000
H	-0.022737000	11.355184000	7.955618000
C	-1.085261000	12.772445000	4.948451000
H	-0.695201000	13.139423000	5.906564000
H	-0.395222000	13.135556000	4.186152000
O	-0.223031000	16.180318000	7.501176000

C	0.597324000	16.016703000	8.457230000
C	0.192816000	15.930223000	9.847256000
O	-1.957381000	15.181986000	9.497072000
N	-1.230167000	15.879750000	10.195906000
C	2.035707000	15.943205000	8.286107000
N	2.620219000	15.909212000	6.944251000
O	2.010528000	15.294249000	6.075601000
O	3.705019000	16.469163000	6.783927000
C	2.931668000	15.883666000	9.342300000
H	4.001215000	15.860698000	9.147682000
C	2.456222000	15.844828000	10.653231000
C	1.082911000	15.874656000	10.906390000
H	0.714263000	15.846529000	11.929116000
O	-1.590333000	16.510443000	11.188612000
N	3.397212000	15.768940000	11.764188000
O	2.930718000	15.734175000	12.902808000
O	4.597681000	15.748710000	11.492814000
O	-3.386917000	10.010365000	2.165450000
C	-4.230054000	10.171575000	1.229002000
C	-3.857891000	10.273497000	-0.168993000
O	-1.706654000	11.037265000	0.139653000
N	-2.443811000	10.340177000	-0.549421000
C	-5.665086000	10.226098000	1.432535000
N	-6.220265000	10.237838000	2.787220000
O	-7.292935000	9.660193000	2.965273000
O	-5.600579000	10.852725000	3.648723000
C	-6.585159000	10.286729000	0.397433000
H	-7.650261000	10.295924000	0.616102000
C	-6.139805000	10.343778000	-0.923306000
C	-4.772335000	10.329655000	-1.207267000
H	-4.427005000	10.370092000	-2.237695000
O	-2.100855000	9.722315000	-1.556218000
N	-7.106184000	10.421357000	-2.012110000
O	-6.665827000	10.469460000	-3.160620000
O	-8.300355000	10.429685000	-1.713528000
C	-3.281971000	15.628694000	5.650528000
C	-4.677777000	15.297433000	5.917752000
C	-5.162937000	16.307330000	6.733673000
C	-4.059376000	17.189524000	7.000444000
C	-4.082880000	18.182581000	7.972069000
H	-5.015395000	18.328358000	8.507537000
C	-2.983370000	18.913617000	8.397291000
C	-2.965602000	19.790309000	9.546516000
C	-1.659063000	20.222350000	9.681143000
C	-0.927815000	19.648220000	8.573669000
C	0.385983000	19.961007000	8.245946000
H	0.940969000	20.597329000	8.927940000
C	0.967067000	19.655852000	7.020381000
C	2.173076000	20.266125000	6.507848000
C	2.257933000	19.893456000	5.178328000
C	1.145112000	19.003555000	4.936980000
C	0.903191000	18.335108000	3.745410000
H	1.558287000	18.553271000	2.907857000
C	-0.024805000	17.314093000	3.578206000
C	-0.083469000	16.467326000	2.418638000
C	-0.932286000	15.418927000	2.734079000
C	-1.432402000	15.689991000	4.072168000
C	-2.404661000	14.941377000	4.778143000
C	-5.544169000	14.237384000	5.292640000
H	-6.334089000	13.968685000	6.009279000
H	-5.003060000	13.307550000	5.107252000
C	-6.205368000	14.676084000	3.977461000
H	-6.820290000	13.858075000	3.578101000
H	-5.455080000	14.934765000	3.220149000
H	-6.850494000	15.552020000	4.118719000
C	-6.551762000	16.486756000	7.274029000
H	-6.495151000	16.650767000	8.362394000
H	-7.112689000	15.550611000	7.152873000
C	-7.353381000	17.631333000	6.637082000
H	-8.352662000	17.696130000	7.091019000
H	-7.482485000	17.476162000	5.558471000
H	-6.856792000	18.601130000	6.771995000
C	-4.147830000	20.114522000	10.410685000

Structure [11]**2**•picrate

Fe	-0.979779000	17.550073000	6.641056000
Fe	-2.590501000	8.711752000	3.085414000
C	-3.309125000	15.630898000	5.912383000
C	-4.695392000	15.294134000	6.206081000
C	-5.144276000	16.286948000	7.067492000
C	-4.025526000	17.173232000	7.299488000
C	-3.999441000	18.201072000	8.238895000
H	-4.909145000	18.341156000	8.817036000
C	-2.922419000	19.031833000	8.577021000
C	-2.925442000	20.010619000	9.647178000
C	-1.657041000	20.565915000	9.666663000
C	-0.927721000	19.941127000	8.579022000
C	0.343491000	20.320828000	8.133953000
H	0.855029000	21.082909000	8.716446000
C	0.949625000	19.938953000	6.930134000
C	2.098062000	20.584845000	6.324956000
C	2.206811000	20.055495000	5.048845000
C	1.154799000	19.065679000	4.929892000
C	0.903911000	18.276183000	3.800167000
H	1.532259000	18.465259000	2.933316000
C	-0.020259000	17.240955000	3.674255000
C	-0.193249000	16.407509000	2.509765000
C	-1.099637000	15.413148000	2.863325000
C	-1.446415000	15.674536000	4.246719000
C	-2.370063000	14.919667000	5.070429000
C	-5.558401000	14.234706000	5.575421000
H	-6.352334000	13.957661000	6.284467000
H	-5.004934000	13.308521000	5.390168000
C	-6.207212000	14.666508000	4.252166000
H	-6.817162000	13.846430000	3.849182000
H	-5.447390000	14.919061000	3.502405000
H	-6.852558000	15.544056000	4.384266000
C	-6.513748000	16.453310000	7.658461000
H	-6.418390000	16.639584000	8.740551000
H	-7.063232000	15.505617000	7.575347000
C	-7.358302000	17.572813000	7.032206000
H	-8.338445000	17.634925000	7.526617000
H	-7.530011000	17.391656000	5.963662000
H	-6.868833000	18.551151000	7.125210000
C	-4.088059000	20.321133000	10.543765000
H	-3.712232000	20.756781000	11.480775000
H	-4.584430000	19.383104000	10.838063000
C	-5.129170000	21.274342000	9.938711000
H	-5.948134000	21.450034000	10.651063000
H	-5.565093000	20.868203000	9.016208000
H	-4.682526000	22.245887000	9.690375000
C	-1.114155000	21.618535000	10.588480000
H	-0.063035000	21.390529000	10.824473000
H	-1.645648000	21.563350000	11.549842000
C	-1.209003000	23.055378000	10.053293000
H	-0.774877000	23.762883000	10.774491000
H	-2.252611000	23.347960000	9.879773000
H	-0.672900000	23.168864000	9.101680000
C	2.960947000	21.623768000	6.977666000
H	2.326987000	22.369338000	7.483683000
H	3.505020000	22.182058000	6.202486000
C	3.973157000	21.057945000	7.985213000
H	4.583375000	21.867177000	8.411612000
H	4.646867000	20.335530000	7.507177000
H	3.472821000	20.538207000	8.813179000
C	3.212280000	20.390300000	3.986410000
H	3.558912000	21.424492000	4.128288000
H	2.722387000	20.382486000	3.000285000
C	4.431200000	19.456414000	3.952426000
H	5.107964000	19.739622000	3.133261000
H	4.133779000	18.409757000	3.807855000
H	4.994313000	19.505258000	4.892776000
C	0.512458000	16.574524000	1.195099000
H	0.663770000	17.643745000	0.982931000
H	-0.129315000	16.202139000	0.385295000
C	1.863111000	15.844579000	1.125929000
H	2.342488000	16.014459000	0.150890000
H	1.732753000	14.761674000	1.253973000
H	2.550237000	16.189873000	1.909918000
C	-1.738539000	14.429418000	1.921110000
H	-2.157470000	13.578641000	2.467959000
H	-0.973638000	14.003030000	1.255992000
C	-2.857008000	15.047843000	1.068562000
H	-3.285753000	14.284756000	0.403551000
H	-2.493964000	15.875709000	0.445451000
H	-3.664477000	15.441184000	1.699631000
C	-2.321350000	13.507596000	5.164594000
H	-3.116631000	13.025608000	5.725731000

N	-2.945570000	16.777824000	6.541132000
N	-1.704911000	18.998942000	7.956535000
N	0.424480000	18.996803000	6.085067000
N	-0.834970000	16.797590000	4.696333000
N	-0.623739000	9.458101000	3.280422000
N	-1.845395000	7.293371000	1.751726000
N	-4.069880000	7.300526000	3.522877000
N	-2.827458000	9.432135000	5.028092000
C	-0.278750000	10.597353000	3.935207000
C	1.108318000	10.953337000	3.660986000
C	1.577709000	9.976284000	2.793712000
C	0.468819000	9.085543000	2.530152000
C	0.465502000	8.077023000	1.568833000
H	1.390895000	7.943626000	1.014646000
C	-0.602029000	7.255259000	1.181975000
C	-0.561574000	6.282879000	0.106672000
C	-1.831037000	5.734455000	0.033224000
C	-2.603178000	6.360528000	1.089786000
C	-3.904159000	6.004327000	1.460979000
H	-4.398518000	5.259709000	0.842218000
C	-4.575076000	6.394867000	2.627352000
C	-5.791193000	5.793942000	3.139993000
C	-5.965428000	6.308601000	4.414884000
C	-4.880292000	7.246071000	4.624424000
C	-4.665965000	7.998239000	5.786733000
H	-5.350984000	7.813915000	6.610698000
C	-3.705740000	8.986249000	5.995538000
C	-3.549513000	9.765163000	7.199218000
C	-2.582806000	10.727604000	6.925817000
C	-2.192429000	10.510419000	5.547539000
C	-1.230819000	11.281231000	4.782360000
C	1.955144000	12.019856000	4.302024000
H	2.858507000	12.156559000	3.691361000
H	1.462823000	12.999673000	4.296009000
C	2.385448000	11.703563000	5.740953000
H	3.029225000	12.506644000	6.125259000
H	1.520185000	11.620606000	6.408755000
H	2.943557000	10.759498000	5.794085000
C	2.958242000	9.820065000	2.227227000
H	2.884318000	9.578623000	1.155137000
H	3.483061000	10.784291000	2.268177000
C	3.817826000	8.754887000	2.923476000
H	4.802774000	8.680557000	2.440392000
H	3.978293000	9.001757000	3.980927000
H	3.344197000	7.764935000	2.883829000
C	0.633938000	5.973481000	-0.745520000
H	0.293687000	5.544760000	-1.699028000
H	1.142840000	6.911950000	-1.015520000
C	1.648093000	5.013999000	-0.105585000
H	2.493970000	4.840731000	-0.786338000
H	2.048389000	5.413388000	0.835869000
H	1.190027000	4.041856000	0.118802000
C	-2.339384000	4.686617000	-0.913109000
H	-3.374449000	4.925813000	-1.202901000
H	-1.759490000	4.733267000	-1.846198000
C	-2.287515000	3.250972000	-0.369035000
H	-2.690941000	2.545345000	-1.109576000
H	-1.257268000	2.948669000	-0.140591000
H	-2.873576000	3.146847000	0.553762000
C	-6.658055000	4.813162000	2.407737000
H	-6.031291000	4.035264000	1.942844000
H	-7.294040000	4.282787000	3.130570000
C	-7.552125000	5.449313000	1.332464000
H	-8.179423000	4.684632000	0.852147000
H	-8.211913000	6.211851000	1.765845000
H	-6.957351000	5.939430000	0.550283000
C	-7.056159000	6.002390000	5.398882000
H	-7.437332000	4.987628000	5.212288000
H	-6.635616000	5.970612000	6.416080000
C	-8.232880000	6.989212000	5.369506000
H	-8.980413000	6.715946000	6.128277000
H	-7.903327000	8.017692000	5.566151000
H	-8.726127000	6.989809000	4.389324000
C	-4.320637000	9.579315000	8.473963000
H	-4.529211000	8.510805000	8.634780000
H	-3.700342000	9.889614000	9.325532000
C	-5.639370000	10.367396000	8.513731000
H	-6.171163000	10.179156000	9.457677000
H	-5.455611000	11.447531000	8.439397000
H	-6.303225000	10.086908000	7.685037000
C	-1.923723000	11.628327000	7.934460000
H	-1.439541000	12.476151000	7.437040000
H	-2.683295000	12.065660000	8.599281000
C	-0.872493000	10.899234000	8.786532000
H	-0.424298000	11.595864000	9.507762000
H	-1.309109000	10.064540000	9.350252000
H	-0.070896000	10.487337000	8.159639000
C	-1.269457000	12.696593000	4.732354000
H	-0.466080000	13.186980000	4.191153000
O	0.007373000	16.252760000	7.765019000
C	0.860122000	15.901243000	8.651075000
C	0.485668000	15.397690000	9.949423000
O	-1.668693000	16.209220000	10.064893000
N	-0.930877000	15.265618000	10.311638000
C	2.287473000	15.920175000	8.444336000
N	2.843953000	16.252144000	7.127681000
O	2.312331000	15.734373000	6.152376000
O	3.831209000	16.982989000	7.102087000
C	3.210792000	15.598181000	9.427273000
H	4.275952000	15.684457000	9.225746000
C	2.763836000	15.130982000	10.663317000
C	1.398308000	14.995339000	10.912354000
H	1.051742000	14.592336000	11.861052000
O	-1.266453000	14.219941000	10.865993000
N	3.730663000	14.760147000	11.694027000
O	3.286433000	14.359215000	12.768330000
O	4.923824000	14.874805000	11.419032000
O	-3.511943000	10.004254000	1.916414000
C	-4.278602000	10.179427000	0.906867000
C	-3.782950000	10.300190000	-0.441526000
O	-1.674556000	11.079627000	0.054014000
N	-2.337093000	10.366538000	-0.690101000
C	-5.716512000	10.228029000	0.999134000
N	-6.378461000	10.216441000	2.309529000
O	-7.442565000	9.605852000	2.394369000
O	-5.846190000	10.846752000	3.215684000
C	-6.547437000	10.305685000	-0.108918000
H	-7.627288000	10.307834000	0.018608000
C	-5.989530000	10.386892000	-1.384503000
C	-4.604314000	10.376207000	-1.554694000
H	-4.173170000	10.431960000	-2.551514000
O	-1.904076000	9.732748000	-1.649518000
N	-6.862686000	10.482342000	-2.552962000
O	-6.325201000	10.554802000	-3.656600000
O	-8.076272000	10.480921000	-2.355044000

Structure ^{1}2•picrate{3/2}

Fe	-1.236139000	17.662703000	6.400113000
Fe	-2.365078000	8.578077000	3.310327000
C	-3.388632000	15.628514000	5.916889000
C	-4.765846000	15.303583000	6.229218000
C	-5.231982000	16.349964000	7.015466000
C	-4.123328000	17.245321000	7.208806000
C	-4.086640000	18.265786000	8.148458000
H	-4.988524000	18.437996000	8.727671000
C	-2.952789000	18.989975000	8.501040000
C	-2.859459000	19.881398000	9.634778000
C	-1.542331000	20.301481000	9.689439000
C	-0.883842000	19.711395000	8.545617000
C	0.396979000	20.035058000	8.111319000
H	0.996802000	20.685712000	8.740162000
C	0.877448000	19.735469000	6.839076000
C	2.009491000	20.375210000	6.209652000
C	1.986935000	19.978962000	4.882981000
C	0.886306000	19.052834000	4.754528000
C	0.554720000	18.357138000	3.596716000
H	1.115682000	18.585685000	2.695443000
C	-0.354648000	17.309788000	3.533063000
C	-0.553002000	16.448441000	2.401793000
C	-1.352238000	15.395828000	2.838223000
C	-1.630538000	15.664065000	4.229330000
C	-2.471937000	14.888594000	5.097038000
C	-5.610009000	14.182139000	5.685938000
H	-6.226340000	13.773306000	6.502093000
H	-4.997432000	13.347737000	5.336676000
C	-6.527877000	14.592281000	4.525162000
H	-7.080681000	13.714988000	4.162767000
H	-5.945300000	14.993210000	3.685830000

H	-7.255908000	15.356022000	4.823605000
C	-6.603804000	16.533936000	7.595642000
H	-6.515823000	16.697075000	8.682600000
H	-7.167417000	15.597538000	7.487461000
C	-7.420185000	17.682109000	6.984070000
H	-8.411697000	17.739057000	7.455735000
H	-7.565964000	17.538391000	5.905878000
H	-6.924942000	18.652220000	7.120295000
C	-3.987741000	20.235987000	10.557806000
H	-3.571587000	20.587520000	11.512640000
H	-4.558974000	19.327680000	10.805395000
C	-4.947507000	21.304288000	10.012934000
H	-5.747361000	21.506955000	10.739548000
H	-5.417217000	20.986699000	9.072556000
H	-4.422635000	22.248156000	9.815308000
C	-0.891560000	21.209418000	10.691427000
H	0.143777000	20.878411000	10.865077000
H	-1.398698000	21.091815000	11.660449000
C	-0.889442000	22.697233000	10.310701000
H	-0.379159000	23.289779000	11.083674000
H	-1.911581000	23.083996000	10.209131000
H	-0.375366000	22.870046000	9.355848000
C	2.971543000	21.305362000	6.887759000
H	2.413464000	22.035264000	7.495699000
H	3.492644000	21.900190000	6.124225000
C	4.016244000	20.606883000	7.770517000
H	4.690738000	21.348141000	8.222615000
H	4.621610000	19.901752000	7.187535000
H	3.546171000	20.036191000	8.582082000
C	2.918640000	20.378117000	3.776701000
H	3.305746000	21.387447000	3.979949000
H	2.354207000	20.469119000	2.835845000
C	4.102593000	19.422339000	3.568260000
H	4.718913000	19.756096000	2.720938000
H	3.763324000	18.398343000	3.366081000
H	4.741486000	19.380424000	4.459172000
C	0.052059000	16.634597000	1.040897000
H	0.151499000	17.707407000	0.817208000
H	-0.634963000	16.238433000	0.280864000
C	1.417516000	15.948763000	0.874873000
H	1.813538000	16.124367000	-0.135765000
H	1.335647000	14.863634000	1.021985000
H	2.150202000	16.326119000	1.600469000
C	-1.982239000	14.351228000	1.958346000
H	-2.293078000	13.478352000	2.539836000
H	-1.238710000	13.976531000	1.240648000
C	-3.205608000	14.876689000	1.191192000
H	-3.622376000	14.079955000	0.559377000
H	-2.957533000	15.727652000	0.543154000
H	-3.992150000	15.206069000	1.882363000
C	-2.382003000	13.475353000	5.220948000
H	-3.151629000	12.986851000	5.811589000
N	-3.037974000	16.830728000	6.466692000
N	-1.746996000	18.896526000	7.852567000
N	0.227259000	18.909916000	5.952782000
N	-1.080459000	16.851493000	4.614555000
N	-0.553479000	9.371133000	3.480862000
N	-1.709639000	7.352680000	1.907133000
N	-3.943419000	7.411402000	3.504357000
N	-2.722548000	9.338626000	5.090752000
C	-0.260560000	10.568696000	4.075291000
C	1.134848000	10.911078000	3.877982000
C	1.678553000	9.868547000	3.138156000
C	0.597756000	8.966457000	2.841689000
C	0.662106000	7.937585000	1.912161000
H	1.623847000	7.752534000	1.443988000
C	-0.426860000	7.216388000	1.434311000
C	-0.384942000	6.299689000	0.317509000
C	-1.692289000	5.911690000	0.085330000
C	-2.490419000	6.549589000	1.108200000
C	-3.840576000	6.305090000	1.332119000
H	-4.370257000	5.686116000	0.614492000
C	-4.505313000	6.651491000	2.505887000
C	-5.777020000	6.110557000	2.926590000
C	-5.934182000	6.482568000	4.251508000
C	-4.791686000	7.301013000	4.581280000
C	-4.571038000	7.914549000	5.810077000
H	-5.267705000	7.693228000	6.613349000
C	-3.594431000	8.870513000	6.054809000
C	-3.464908000	9.642526000	7.258479000
C	-2.554302000	10.658176000	6.980535000
C	-2.153909000	10.463816000	5.608854000
C	-1.234324000	11.273206000	4.856292000
C	1.924185000	12.037868000	4.487300000
H	2.724490000	12.320395000	3.787244000
H	1.323817000	12.943062000	4.611810000
C	2.552421000	11.696130000	5.845771000
H	3.122848000	12.556386000	6.221709000
H	1.783520000	11.452547000	6.589142000
H	3.234102000	10.839629000	5.774569000
C	3.099724000	9.683847000	2.693414000
H	3.113784000	9.461575000	1.614081000
H	3.639481000	10.634318000	2.800473000
C	3.872778000	8.586340000	3.439693000
H	4.899450000	8.513029000	3.053230000
H	3.931610000	8.799605000	4.514689000
H	3.397112000	7.603428000	3.325022000
C	0.852608000	5.895157000	-0.427358000
H	0.567363000	5.528463000	-1.423402000
H	1.475892000	6.783764000	-0.612427000
C	1.695144000	4.820893000	0.275704000
H	2.583213000	4.575788000	-0.324418000
H	2.036786000	5.154947000	1.264520000
H	1.119914000	3.897128000	0.421421000
C	-2.219646000	4.996412000	-0.980103000
H	-3.196082000	5.366456000	-1.328522000
H	-1.559710000	5.054840000	-1.857801000
C	-2.356422000	3.526239000	-0.557762000
H	-2.765422000	2.927235000	-1.384112000
H	-1.384139000	3.098813000	-0.280385000
H	-3.024734000	3.413781000	0.306319000
C	-6.703316000	5.295568000	2.073856000
H	-6.137034000	4.502731000	1.559105000
H	-7.417274000	4.769984000	2.723298000
C	-7.486171000	6.113625000	1.035823000
H	-8.176395000	5.464327000	0.478546000
H	-8.072890000	6.907097000	1.516246000
H	-6.817358000	6.596347000	0.311205000
C	-7.062292000	6.149944000	5.183260000
H	-7.506812000	5.190654000	4.880374000
H	-6.664636000	5.976693000	6.195273000
C	-8.168103000	7.213768000	5.248288000
H	-8.949003000	6.909447000	5.960085000
H	-7.773711000	8.187576000	5.565875000
H	-8.637872000	7.359582000	4.267447000
C	-4.225346000	9.412778000	8.532114000
H	-4.422135000	8.338115000	8.662607000
H	-3.599437000	9.703609000	9.386589000
C	-5.550153000	10.188003000	8.607269000
H	-6.070017000	9.968536000	9.551040000
H	-5.377295000	11.271399000	8.561476000
H	-6.219984000	9.924773000	7.777917000
C	-1.935043000	11.590539000	7.985334000
H	-1.484526000	12.454449000	7.485018000
H	-2.712789000	11.998198000	8.647777000
C	-0.855581000	10.907228000	8.840025000
H	-0.437573000	11.624721000	9.558358000
H	-1.256127000	10.056347000	9.406180000
H	-0.037700000	10.528383000	8.213403000
C	-1.321346000	12.690566000	4.780957000
H	-0.543805000	13.191359000	4.211365000
O	-0.205258000	16.219873000	7.516681000
C	0.682433000	15.894831000	8.363064000
C	0.379905000	15.419905000	9.700800000
O	-1.812273000	16.130088000	9.835225000
N	-1.011283000	15.254384000	10.132700000
C	2.109405000	15.907531000	8.094601000
N	2.610158000	16.173685000	6.744400000
O	1.994880000	15.675476000	5.807807000
O	3.643918000	16.833426000	6.641805000
C	3.077419000	15.634649000	9.048057000
H	4.131186000	15.718656000	8.792803000
C	2.694708000	15.216567000	10.323298000
C	1.342320000	15.068782000	10.633822000
H	1.044201000	14.693769000	11.610101000
O	-1.274271000	14.246410000	10.791257000
N	3.708778000	14.904748000	11.321668000
O	3.320778000	14.539059000	12.431262000
O	4.888678000	15.028599000	10.992488000
O	-3.196097000	10.046810000	2.106799000

C	-3.939283000	10.257521000	1.098448000
C	-3.437890000	10.309699000	-0.260617000
O	-1.286423000	10.965865000	0.226826000
N	-1.993154000	10.286970000	-0.509640000
C	-5.377023000	10.426116000	1.175398000
N	-6.040446000	10.523786000	2.476890000
O	-7.174342000	10.052667000	2.572813000
O	-5.439529000	11.101955000	3.376061000
C	-6.196248000	10.525078000	0.061034000
H	-7.272591000	10.618116000	0.184234000
C	-5.634008000	10.513358000	-1.215897000
C	-4.250800000	10.401549000	-1.377366000
H	-3.814514000	10.397388000	-2.373594000
O	-1.595824000	9.620816000	-1.464340000
N	-6.493870000	10.625737000	-2.387761000
O	-5.953022000	10.606801000	-3.493433000
O	-7.705640000	10.727884000	-2.197325000

Structure [7]**2•**picrate

Fe	-1.231824000	17.659488000	6.410556000
Fe	-2.367802000	8.561841000	3.300133000
C	-3.376306000	15.610864000	5.938710000
C	-4.751658000	15.282050000	6.256793000
C	-5.215110000	16.322834000	7.051718000
C	-4.107734000	17.220007000	7.242904000
C	-4.069529000	18.235808000	8.187668000
H	-4.967677000	18.399348000	8.775118000
C	-2.937790000	18.966040000	8.533552000
C	-2.840763000	19.854704000	9.668906000
C	-1.526921000	20.286746000	9.711009000
C	-0.875217000	19.706665000	8.558140000
C	0.395785000	20.047937000	8.108565000
H	0.995211000	20.705037000	8.730992000
C	0.863101000	19.757943000	6.829237000
C	1.976540000	20.416337000	6.185849000
C	1.944712000	20.019246000	4.859574000
C	0.858618000	19.074489000	4.744793000
C	0.528456000	18.369278000	3.592669000
H	1.079316000	18.602084000	2.686356000
C	-0.365378000	17.307838000	3.540218000
C	-0.557321000	16.439176000	2.413553000
C	-1.343746000	15.379858000	2.856329000
C	-1.622206000	15.651089000	4.247569000
C	-2.460898000	14.874840000	5.115271000
C	-5.600275000	14.165883000	5.709482000
H	-6.217788000	13.756297000	6.524272000
H	-4.992309000	13.330153000	5.355892000
C	-6.517275000	14.585109000	4.551215000
H	-7.072687000	13.711394000	4.184163000
H	-5.933633000	14.988705000	3.713925000
H	-7.242784000	15.349568000	4.853952000
C	-6.583937000	16.501288000	7.640708000
H	-6.489746000	16.658293000	8.728071000
H	-7.146730000	15.564630000	7.530593000
C	-7.406075000	17.651521000	7.040862000
H	-8.394470000	17.704337000	7.519496000
H	-7.558970000	17.513476000	5.962934000
H	-6.911373000	18.621609000	7.179001000
C	-3.962954000	20.196988000	10.604001000
H	-3.540571000	20.550983000	11.555171000
H	-4.522989000	19.282817000	10.855593000
C	-4.938186000	21.256957000	10.070512000
H	-5.733056000	21.450473000	10.805060000
H	-5.413613000	20.936610000	9.133989000
H	-4.424458000	22.206261000	9.869778000
C	-0.874312000	21.197615000	10.709128000
H	0.166995000	20.878281000	10.867980000
H	-1.367666000	21.069044000	11.683912000
C	-0.895060000	22.687226000	10.336112000
H	-0.381654000	23.281932000	11.105345000
H	-1.922998000	23.062159000	10.250137000
H	-0.395857000	22.871020000	9.375443000
C	2.930172000	21.364367000	6.850984000
H	2.366647000	22.085679000	7.464138000
H	3.431513000	21.966552000	6.080046000
C	3.998086000	20.687006000	7.722435000
H	4.665688000	21.441524000	8.162649000
H	4.607626000	19.989929000	7.134178000
H	3.548813000	20.111742000	8.542497000
C	2.855976000	20.434145000	3.742164000
H	3.225353000	21.451322000	3.939285000
H	2.279419000	20.512335000	2.807557000
C	4.056443000	19.501770000	3.522000000
H	4.658031000	19.848041000	2.669140000
H	3.735643000	18.471352000	3.322222000
H	4.704358000	19.471923000	4.406881000
C	0.040641000	16.627199000	1.049712000
H	0.125052000	17.700208000	0.820876000
H	-0.643447000	16.218572000	0.293687000
C	1.414677000	15.959100000	0.882068000
H	1.805798000	16.137357000	-0.130016000
H	1.347731000	14.873309000	1.031904000
H	2.144095000	16.347981000	1.604849000
C	-1.965054000	14.327707000	1.979094000
H	-2.264874000	13.451710000	2.561381000
H	-1.219082000	13.961556000	1.259383000
C	-3.195949000	14.839778000	1.214893000
H	-3.603974000	14.039209000	0.582297000
H	-2.959475000	15.695076000	0.568229000
H	-3.985232000	15.157861000	1.908143000
C	-2.373464000	13.458557000	5.229645000
H	-3.153837000	12.963896000	5.800435000
N	-3.026035000	16.812728000	6.491490000
N	-1.737681000	18.884871000	7.872871000
N	0.215581000	18.922408000	5.950622000
N	-1.082102000	16.846202000	4.626066000
N	-0.555053000	9.352937000	3.476904000
N	-1.708437000	7.320770000	1.911701000
N	-3.958571000	7.409532000	3.482336000
N	-2.733582000	9.330751000	5.072943000
C	-0.264174000	10.559586000	4.057339000
C	1.128087000	10.908983000	3.838389000
C	1.671747000	9.856550000	3.113316000
C	0.594599000	8.942426000	2.840360000
C	0.666013000	7.891202000	1.936398000
H	1.631833000	7.692503000	1.482612000
C	-0.419869000	7.163770000	1.461948000
C	-0.369390000	6.226032000	0.363110000
C	-1.677260000	5.849744000	0.114900000
C	-2.485059000	6.513309000	1.113738000
C	-3.841383000	6.287111000	1.319216000
H	-4.367790000	5.666380000	0.600674000
C	-4.517769000	6.652136000	2.480693000
C	-5.801539000	6.129991000	2.888633000
C	-5.968800000	6.508513000	4.210610000
C	-4.819539000	7.312993000	4.550425000
C	-4.601217000	7.924422000	5.780360000
H	-5.306153000	7.711938000	6.578750000
C	-3.614957000	8.869042000	6.031431000
C	-3.482699000	9.635438000	7.238059000
C	-2.559644000	10.641722000	6.968194000
C	-2.155350000	10.449299000	5.596671000
C	-1.230509000	11.257630000	4.850838000
C	1.922017000	12.049689000	4.414311000
H	2.830509000	12.171534000	3.808183000
H	1.398395000	13.007657000	4.326499000
C	2.336663000	11.852254000	5.878725000
H	2.960866000	12.693374000	6.207888000
H	1.463186000	11.806172000	6.539130000
H	2.910775000	10.926127000	6.012400000
C	3.092198000	9.663761000	2.670146000
H	3.103751000	9.348495000	1.615012000
H	3.614618000	10.629688000	2.686308000
C	3.889623000	8.652900000	3.507027000
H	4.913311000	8.556571000	3.117651000
H	3.955847000	8.969656000	4.555956000
H	3.425498000	7.657683000	3.490676000
C	0.875935000	5.793067000	-0.352207000
H	0.603025000	5.403097000	-1.342848000
H	1.509419000	6.671683000	-0.550189000
C	1.698734000	4.730787000	0.391187000
H	2.592386000	4.461494000	-0.189948000
H	2.030194000	5.088638000	1.375117000
H	1.112787000	3.816641000	0.553913000
C	-2.197497000	4.922567000	-0.943673000
H	-3.166417000	5.294532000	-1.310398000

H	-1.525751000	4.962730000	-1.813402000
C	-2.351040000	3.460153000	-0.500729000
H	-2.754207000	2.851625000	-1.322977000
H	-1.385645000	3.029729000	-0.204533000
H	-3.031021000	3.366179000	0.356450000
C	-6.729182000	5.325352000	2.027728000
H	-6.168148000	4.523146000	1.521876000
H	-7.458113000	4.811871000	2.670190000
C	-7.487651000	6.151723000	0.978266000
H	-8.179811000	5.510904000	0.413635000
H	-8.069331000	6.954245000	1.449794000
H	-6.802928000	6.623476000	0.261316000
C	-7.110880000	6.192864000	5.131123000
H	-7.565036000	5.239005000	4.825404000
H	-6.725879000	6.016319000	6.147444000
C	-8.203004000	7.271469000	5.183145000
H	-8.994263000	6.979634000	5.888711000
H	-7.798508000	8.240880000	5.501473000
H	-8.662104000	7.420611000	4.197751000
C	-4.250656000	9.407627000	8.507630000
H	-4.457545000	8.334218000	8.632749000
H	-3.625880000	9.689184000	9.365946000
C	-5.568894000	10.194103000	8.580803000
H	-6.095039000	9.974141000	9.520978000
H	-5.386273000	11.276121000	8.541807000
H	-6.237261000	9.941268000	7.747054000
C	-1.937533000	11.563031000	7.981394000
H	-1.476472000	12.425433000	7.488326000
H	-2.715800000	11.975116000	8.640536000
C	-0.871022000	10.864574000	8.840477000
H	-0.445829000	11.576619000	9.560163000
H	-1.286191000	10.020140000	9.405726000
H	-0.055999000	10.473265000	8.217809000
C	-1.306745000	12.679369000	4.800574000
H	-0.513817000	13.187902000	4.261024000
O	-0.175603000	16.225989000	7.509596000
C	0.724569000	15.916603000	8.348983000
C	0.440781000	15.431762000	9.687025000
O	-1.767208000	16.089488000	9.833456000
N	-0.943682000	15.233577000	10.126888000
C	2.148935000	15.959611000	8.070624000
N	2.634923000	16.233911000	6.716421000
O	2.024791000	15.719444000	5.785314000
O	3.653368000	16.915663000	6.605704000
C	3.128712000	15.707147000	9.017634000
H	4.178775000	15.813994000	8.755743000
C	2.763303000	15.279550000	10.294853000
C	1.416628000	15.100529000	10.613428000
H	1.133012000	14.717039000	11.590722000
O	-1.178655000	14.219933000	10.787344000
N	3.790489000	14.989923000	11.286565000
O	3.418019000	14.612892000	12.397649000
O	4.965063000	15.142744000	10.950625000
O	-3.178138000	10.029240000	2.084074000
C	-3.914970000	10.241204000	1.071152000
C	-3.408783000	10.271230000	-0.286544000
O	-1.252120000	10.910567000	0.197755000
N	-1.963493000	10.227098000	-0.529844000
C	-5.349842000	10.433548000	1.142095000
N	-6.014754000	10.557077000	2.440521000
O	-7.157366000	10.107901000	2.538391000
O	-5.405520000	11.133739000	3.335059000
C	-6.164293000	10.532509000	0.024146000
H	-7.239348000	10.643921000	0.143195000
C	-5.598745000	10.496613000	-1.250789000
C	-4.216817000	10.362047000	-1.406801000
H	-3.777730000	10.340076000	-2.401584000
O	-1.570681000	9.540363000	-1.471622000
N	-6.453429000	10.607985000	-2.426579000
O	-5.909896000	10.565361000	-3.530255000
O	-7.663806000	10.732981000	-2.241091000